

Electronic Supplementary Data

On Calculating Polymeric Binders' Enthalpy of Formations and Band Gaps with Computational Methods

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Cartesian coordinates of all B3LYP/6-31G(d) optimized stationary points of monomer, dimer, trimer tetramer and pentamers of HTPB, GAP and AHTPB in the gas phase, including corresponding charge and multiplicity were given.

Monomer of HTPB

Charge = 0; Multiplicity = 1

C	-0.56300300	-0.15713400	0.32174200
H	-0.57208800	-0.97227800	1.04580700
C	0.56277400	0.15722900	-0.32033300
H	0.57185700	0.97238700	-1.04438100
C	1.87224100	-0.54903000	-0.13742800
H	1.78624600	-1.30346700	0.66071000
C	-1.87251000	0.54894600	0.13848900
H	-1.78572800	1.30503000	-0.65800000
H	-2.13044300	1.08191700	1.07033500
O	-2.87082100	-0.42587300	-0.16806500
H	-3.73215200	0.01769700	-0.13453400
O	2.87135400	0.42597100	0.16573700
H	3.73242400	-0.01810800	0.13242700
H	2.12861100	-1.08402600	-1.06855200

Dimer of HTPB

Charge = 0; Multiplicity = 1

C	0.54523900	0.47963500	0.26968800
H	0.22235600	0.84815700	1.25412800
H	0.61993200	1.35682500	-0.38606800
C	4.31207800	-0.52211000	-0.17251300
H	4.55197800	-0.99621300	-1.14060800
H	4.25582400	-1.32584300	0.57943100
C	2.99020900	0.17716500	-0.27417800
H	2.96530900	1.02883800	-0.95491500
C	1.89039200	-0.18068500	0.39247600
H	1.94378100	-1.03021900	1.07742900
C	-0.54520400	-0.47928800	-0.26935700
H	-0.22234600	-0.84776200	-1.25382300
H	-0.61985400	-1.35651000	0.38636100
C	-1.89038800	0.18101100	-0.39207300
H	-1.94366700	1.03087100	-1.07664200
C	-2.99025300	-0.17724800	0.27424800
H	-2.96539400	-1.02927600	0.95452400
C	-4.31222400	0.52185900	0.17259100
H	-4.55254100	0.99538900	1.14087100
H	-4.25585700	1.32603600	-0.57887300
O	-5.31021400	-0.44326900	-0.16554600
H	-6.17446200	-0.01330800	-0.07545700
O	5.31038100	0.44304200	0.16473500
H	6.17451000	0.01279400	0.07484000

Trimer of HTPB

Charge = 0; Multiplicity = 1

C	-1.89530700	-0.46888200	-0.24735600
H	-2.20948700	-0.80606100	-1.24607400
H	-1.83016300	-1.36753200	0.38036800
C	1.89530800	0.46888300	0.24735700
H	2.20948800	0.80606100	1.24607500
H	1.83016300	1.36753400	-0.38036500

C	0.54698300	-0.19286600	0.33142600
H	0.48603300	-1.06896500	0.98181300
C	-0.54698300	0.19286600	-0.33142500
H	-0.48603300	1.06896600	-0.98181200
C	-2.99109700	0.47289500	0.31049400
H	-2.67802800	0.80915600	1.30948900
H	-3.05757300	1.37099200	-0.31727700
C	2.99109600	-0.47289400	-0.31049400
H	3.05757200	-1.37099100	0.31727500
H	2.67802700	-0.80915300	-1.30949000
C	4.33814200	0.18903900	-0.39786900
H	4.39979700	1.05931000	-1.05568200
C	5.43081000	-0.18994500	0.26895300
H	5.39851900	-1.06225300	0.92271900
C	-4.33814200	-0.18903800	0.39786900
H	-4.39979700	-1.05930800	1.05568300
C	-5.43081000	0.18994500	-0.26895400
H	-5.39851900	1.06225200	-0.92272100
C	6.75387000	0.51129300	0.20219300
H	6.70499200	1.33815600	-0.52479500
H	6.98486500	0.95474000	1.18687100
C	-6.75387000	-0.51129400	-0.20219300
H	-6.98486500	-0.95474200	-1.18687100
H	-6.70499100	-1.33815600	0.52479600
O	-7.75537500	0.44318400	0.15560400
H	-8.61857200	0.01609900	0.04417900
O	7.75537500	-0.44318500	-0.15560500
H	8.61857200	-0.01610000	-0.04418000

Tetramer of HTPB

Charge = 0; Multiplicity = 1

C	4.32269400	-0.49943700	-0.12225300
H	4.65977500	-1.39132900	0.42621100
H	4.26033400	-0.78760900	-1.18009500
C	0.50952200	0.44854800	0.11365900
H	0.17131300	1.33943800	-0.43547600
H	0.57135700	0.73785900	1.17119000
C	1.86658900	0.02721000	-0.37995100
H	1.93020600	-0.22539900	-1.44137500
C	2.96606700	-0.07702300	0.37190700
H	2.90308200	0.17575200	1.43324200
C	5.39418900	0.60570600	0.04976800
H	5.05967300	1.49643700	-0.50130200
H	5.45634700	0.89484900	1.10696300
C	-0.56096800	-0.65754000	-0.05706600
H	-0.62257600	-0.94672300	-1.11466500
H	-0.22247900	-1.54848500	0.49197500
C	-1.91843300	-0.23693000	0.43620500
H	-1.98270600	0.01536000	1.49765800
C	-3.01744000	-0.13293300	-0.31639700
H	-2.95312200	-0.38457600	-1.37794400
C	6.75003100	0.18360000	-0.44396200
H	6.81591000	-0.05970600	-1.50716400
C	7.84602000	0.06915400	0.30964500
H	7.80925400	0.31736700	1.37097900

C	-4.37488000	0.28841300	0.17633700
H	-4.31419900	0.57656200	1.23425500
H	-4.71314600	1.17922400	-0.37249000
C	9.17844900	-0.39869500	-0.19271600
H	9.42919100	-1.36607700	0.27728300
H	9.13231800	-0.56691500	-1.28095300
O	10.16095700	0.58245800	0.14511900
H	11.03168900	0.20103200	-0.04529100
C	-5.44385000	-0.81856200	0.00318600
H	-5.50275100	-1.11063700	-1.05344000
H	-5.10888100	-1.70825800	0.55637000
C	-6.80124600	-0.39449200	0.49098300
H	-6.86473600	-0.12166400	1.54716400
C	-7.90281600	-0.31769800	-0.25915000
H	-7.86190300	-0.56926200	-1.31953300
C	-9.25336500	0.08350500	0.25215100
H	-9.94006000	-0.77941300	0.19404500
H	-9.18321800	0.37342700	1.31318600
O	-9.74253900	1.15761600	-0.55372600
H	-10.67140100	1.30120400	-0.31600900

Pentamer of HTPB

Charge = 0; Multiplicity = 1

C	-6.76877300	-0.45341500	-0.23091800
H	-7.06625500	-0.82626500	-1.22209000
H	-6.68746000	-1.33230200	0.42241800
C	-3.00148200	0.57331100	0.27006500
H	-2.69494700	0.92046700	1.26763500
H	-3.07974600	1.46744500	-0.36253100
C	-4.33821600	-0.111108400	0.35662000
H	-4.38692700	-0.97504000	1.02420700
C	-5.43531500	0.23732500	-0.32157200
H	-5.38921100	1.10057100	-0.99006100
C	-7.89243500	0.47587500	0.29128400
H	-7.59125500	0.85778600	1.27740800
H	-7.98462300	1.34765900	-0.36938600
C	-1.88985100	-0.35354000	-0.28096400
H	-1.83113500	-1.26065100	0.33524300
H	-2.18597800	-0.67931800	-1.28898400
C	-0.54237700	0.31355100	-0.33133600
H	-0.47533800	1.20929400	-0.95390200
C	0.54476000	-0.09310800	0.33037100
H	0.47533600	-0.98972300	0.95145100
C	-9.21903400	-0.22274100	0.40279100
H	-9.25617200	-1.06623000	1.09636700
C	-10.32042400	0.09307000	-0.28231300
H	-10.31328900	0.93761600	-0.97226200
C	1.89607600	0.56595800	0.28318500
H	1.83814800	1.49653900	-0.29700700
H	2.20922500	0.84866900	1.29889800
C	-11.62057000	-0.64699700	-0.18950000
H	-11.83348300	-1.13841200	-1.15532000
H	-11.54784600	-1.44097500	0.57142700
O	-12.65368000	0.28859500	0.12579600
H	-13.50221200	-0.17066300	0.03093700

C	2.98798500	-0.35153900	-0.32055000
H	3.02766900	-1.29322200	0.24306800
H	2.68508500	-0.61348500	-1.34498900
C	4.34889300	0.28916300	-0.33541200
H	4.43460900	1.21564700	-0.90881600
C	5.42763100	-0.17488000	0.30182300
H	5.34108700	-1.10189000	0.87408000
C	6.79107800	0.46037900	0.28678600
H	6.74941400	1.42042400	-0.24480500
H	7.11038100	0.68494900	1.31507200
C	7.86521900	-0.44519800	-0.36540400
H	7.55278600	-0.65742700	-1.39807200
H	7.89818400	-1.41011900	0.15713400
C	9.23258400	0.17966600	-0.36698900
H	9.32825800	1.11798800	-0.91864500
C	10.30599000	-0.31033300	0.25748700
H	10.23892100	-1.25138300	0.80463900
C	11.65117500	0.35015300	0.28226000
H	11.88618500	0.66678200	1.31383900
H	11.63606500	1.25822300	-0.34219500
O	12.62572000	-0.58765600	-0.17916500
H	13.50071100	-0.20415400	-0.01409900

Monomer of GAP

Charge = 0; Multiplicity = 1

C	0.68511800	0.34033600	-0.29962900
H	0.72078400	0.18686600	-1.38739600
C	-0.06883800	-0.83136300	0.32586800
H	-0.19107000	-0.64720600	1.40233300
H	0.51159600	-1.74497000	0.19144000
N	-1.37173300	-1.07527600	-0.32042600
N	-2.28592800	-0.29342700	-0.03221200
N	-3.22921700	0.32451300	0.14653400
C	2.11650400	0.44346100	0.23337700
H	2.57798800	1.35658900	-0.17760500
H	2.08256300	0.55423100	1.32858200
O	2.82119400	-0.72488900	-0.16510100
H	3.70911800	-0.69073100	0.22026400
O	-0.04027500	1.52219800	0.03235300
H	0.15311500	2.20147800	-0.63059600

Dimer of GAP

Charge = -1; Multiplicity = 1

C	-1.01043500	0.79290000	-0.37851400
C	-1.34038900	1.94494000	0.56937100
H	-0.39733100	2.41512900	0.88359800
H	-1.83974900	1.53937200	1.45982300
O	-2.17325500	2.85307600	-0.14219400
H	-2.48924200	3.52254300	0.48181400
O	-0.09500200	-0.03096400	0.32300500
C	0.56786200	-1.01413300	-0.45584900
H	-0.11394000	-1.81688700	-0.76614600
H	1.01798300	-0.56927100	-1.35495600
C	1.66350400	-1.62759400	0.41269900
H	1.19232200	-2.00596800	1.33521800

C	2.71476300	-0.60529700	0.84991100
H	2.21718000	0.18930700	1.41787100
H	3.44574200	-1.09183800	1.51387200
O	2.20740800	-2.68707600	-0.35817400
H	2.97080800	-3.05221700	0.11482200
N	3.41533300	-0.06285200	-0.33607800
N	3.96370800	1.03058300	-0.17710900
N	4.50939300	2.03498600	-0.15914600
C	-2.26575500	0.04912200	-0.84483000
H	-2.93524000	0.77712500	-1.31665200
H	-2.00410400	-0.71211800	-1.59103500
N	-2.91300600	-0.59826200	0.31965600
N	-4.08900200	-0.93313500	0.15887800
N	-5.17522300	-1.28928500	0.13735100
H	-0.53335900	1.21065800	-1.28091400

Trimer of GAP

Charge = 0; Multiplicity = 1

C	-2.96800600	0.18635900	0.53182700
C	-4.13982600	0.78377900	-0.24542200
H	-4.20802500	0.28576900	-1.22221800
H	-3.93573400	1.85118400	-0.41290000
O	-5.31086300	0.58479400	0.53803200
H	-6.07576100	0.85217800	0.00799100
C	-3.15331200	-1.30993900	0.80255300
H	-4.08960400	-1.44183100	1.35601200
H	-2.33038500	-1.68990100	1.42180700
H	-2.91105900	0.68638800	1.51286200
O	-1.80859200	0.47451200	-0.23314200
C	-0.57630000	0.36027000	0.45764200
H	-0.57992900	0.97014200	1.37260100
H	-0.35673500	-0.68030500	0.73254100
C	0.52771400	0.85087400	-0.47985500
O	1.73950400	0.65532600	0.22941000
C	2.92142300	0.70010100	-0.55517200
H	3.11633000	1.70868600	-0.94335700
H	2.85736600	0.00480800	-1.40426100
C	4.08843400	0.30288700	0.34567000
H	4.08457800	0.97401500	1.22078400
O	5.25253100	0.49295000	-0.44229900
H	6.01656000	0.15418600	0.04895200
C	3.95953000	-1.12106000	0.89012000
H	3.02889400	-1.19438200	1.46499500
H	4.79780800	-1.32986500	1.57265400
N	3.98016000	-2.09082800	-0.22764400
N	3.52608600	-3.20876000	0.03005400
N	3.13353100	-4.27645300	0.14152000
N	-3.18133200	-2.04322700	-0.48380200
N	-3.73465400	-3.14533200	-0.45798800
N	-4.21834600	-4.17547100	-0.56609800
C	0.31808600	2.30092600	-0.92580900
H	1.09765300	2.59410200	-1.64067000
H	-0.65216500	2.36661000	-1.43092300
N	0.36658700	3.18966700	0.25756900
N	-0.10586400	4.31758500	0.09684000

N	-0.51186200	5.38611800	0.07638000
H	0.51296700	0.22926400	-1.39001000

Tetramer of GAP

Charge = 0; Multiplicity = 1

C	4.71200800	0.67735200	-0.40249100
C	5.66998200	1.57494600	0.37915400
H	5.78172800	1.17341500	1.39559600
H	5.22563900	2.57833500	0.44852200
O	6.90491100	1.59033600	-0.32716500
H	7.55442800	2.06262600	0.21370800
C	5.23897700	-0.75456500	-0.53809100
H	6.21904400	-0.71019400	-1.02586800
H	4.56712900	-1.35043500	-1.16944800
H	4.61202200	1.08058500	-1.42394000
O	3.46933300	0.75574600	0.27760400
C	2.34770800	0.26861900	-0.43880500
H	2.28499400	0.73022700	-1.43480800
H	2.38358800	-0.82237000	-0.55985500
C	1.09606800	0.62142200	0.36561000
O	0.00694200	0.07955600	-0.36530100
C	-1.17552600	-0.14714200	0.38398400
H	-1.59320400	0.78807400	0.78134500
H	-0.98284700	-0.82793700	1.22539300
C	-2.20740300	-0.77078200	-0.55629800
H	-2.38222600	-0.07373500	-1.39205500
O	-3.38539300	-0.91352000	0.21918900
C	-1.72270900	-2.08839600	-1.16809700
H	-0.79332000	-1.88993800	-1.71421500
H	-2.46403100	-2.47069600	-1.88168900
C	-4.57611700	-1.15158000	-0.51591400
H	-4.57604200	-2.14569000	-0.98224400
H	-4.71173000	-0.39582900	-1.30262900
C	-5.74500200	-1.08420300	0.46416000
O	-6.88953600	-1.44383000	-0.29260500
H	-7.67562500	-1.32864700	0.26295100
N	-1.50706700	-3.07814500	-0.08861600
N	-0.86795400	-4.08365200	-0.40872000
N	-0.29161900	-5.05602200	-0.57886900
N	5.33359200	-1.37353700	0.80403400
N	6.10832000	-2.32885500	0.89791000
N	6.79075700	-3.21968000	1.11570100
C	0.95682900	2.12726600	0.60714400
H	0.06431200	2.33197700	1.21270900
H	1.83577300	2.46835000	1.16559400
N	0.84578800	2.82503200	-0.69379200
N	1.08960400	4.03409400	-0.67221500
N	1.29139200	5.15363800	-0.78429500
H	1.17042300	0.13979500	1.35371200
C	-5.87679600	0.28393600	1.13628500
H	-4.95083100	0.49697100	1.68298000
H	-6.70283700	0.25677900	1.86347700
N	-6.15195000	1.32203100	0.11785400
N	-5.88525100	2.47913700	0.45258200
N	-5.67991900	3.58777500	0.64079400

H -5.55442400 -1.81192200 1.27058100

Pentamer of GAP

Charge = 0; Multiplicity = 1

C -2.96721300 0.70530000 -0.36904900
C -4.07413400 0.06125600 0.46698700
H -4.05507600 0.47902900 1.48397800
H -3.87806300 -1.01754100 0.52693700
O -5.30903100 0.33447200 -0.17272500
C -3.13728500 2.22178000 -0.49775400
H -4.11724000 2.41651700 -0.94806200
H -2.36728800 2.63662300 -1.16103900
H -3.01255100 0.28837400 -1.38851000
O -1.75365200 0.32876500 0.26082900
C -0.57501000 0.54572000 -0.49735500
H -0.66212600 0.09954100 -1.49839100
H -0.35320100 1.61557600 -0.60747400
C 0.58367900 -0.10818700 0.25641700
O 1.75026000 0.19614600 -0.49246800
C 2.96705800 0.13997600 0.23384200
H 3.17389800 -0.87242400 0.60722000
H 2.94437900 0.82910800 1.09026400
C 4.09684700 0.54264700 -0.71404400
H 4.13137400 -0.18094000 -1.54414300
O 5.28441300 0.46499300 0.05777700
C 3.88289900 1.92713200 -1.33292700
H 2.95249000 1.90756100 -1.91109500
H 4.70803700 2.16355400 -2.01704900
C 6.48304600 0.29759300 -0.68408500
H 6.68099200 1.15450500 -1.34197700
H 6.44015400 -0.61167500 -1.30016300
C 7.63208200 0.18353700 0.31471300
O 8.80741000 0.10074900 -0.47508500
H 9.56441200 -0.04443700 0.11295300
N 3.82539500 2.94551800 -0.25942200
N 3.22858700 3.98654800 -0.54443800
N 2.70310400 4.99212100 -0.68469400
N -3.02972200 2.84208900 0.84208700
N -3.46494300 3.99312400 0.93253400
N -3.83304200 5.05389200 1.14609400
C -6.47091300 0.02768600 0.58069400
C -7.63438600 0.67042800 -0.17253700
H -7.72113800 0.19923900 -1.16107400
H -7.40771400 1.73699700 -0.31466500
O -8.80366600 0.47778400 0.61491700
H -9.56673800 0.77124700 0.09620800
C 7.46868700 -0.99967300 1.27175600
H 8.30723700 -1.01012600 1.98458400
H 6.54159600 -0.86670600 1.84076700
C 0.38415800 -1.61324100 0.45401900
H 1.22092300 -2.03365600 1.02712400
H -0.53593500 -1.76539000 1.03003900
C -6.67917300 -1.47437700 0.79621300
H -5.87461900 -1.88605500 1.41936500
H -7.62813200 -1.61077000 1.32685500

N	7.45994600	-2.27054600	0.51296000
N	6.84727700	-3.20173900	1.04111100
N	6.31159200	-4.13677200	1.42274300
N	0.29955400	-2.27121100	-0.86892100
N	-0.11214100	-3.43445700	-0.85890300
N	-0.47775800	-4.51012800	-0.98294700
N	-6.69168000	-2.16243300	-0.51503200
N	-7.22403700	-3.27530400	-0.52805000
N	-7.68830800	-4.30985400	-0.67195700
H	-6.40719200	0.48800600	1.58095700
H	0.64371200	0.34646900	1.25805900
H	7.63312100	1.09270800	0.93887800

Monomer of AHTPB

Charge = 0; Multiplicity = 1

C	1.08553100	1.60672000	0.26708100
H	0.36545300	2.31142800	-0.16882900
H	1.01761600	1.66605600	1.36431900
C	-1.08553600	-1.60669300	-0.26683700
H	-0.36559300	-2.31145100	0.16926100
H	-1.01741400	-1.66613800	-1.36404800
O	2.40795700	1.85062000	-0.19191100
H	2.72438000	2.67512400	0.20519300
O	-2.40807600	-1.85046400	0.19191700
H	-2.72464900	-2.67473800	-0.20554700
C	-0.72486000	-0.18734500	0.17599700
H	-0.85599900	-0.12888400	1.26569200
C	0.72491200	0.18732700	-0.17585700
H	0.85576400	0.12911600	-1.26562300
N	1.58995700	-0.80674400	0.49997600
N	2.75122400	-0.90804300	0.08492200
N	-1.58994700	0.80663900	-0.50029600
N	-2.75106100	0.90822300	-0.08482400
N	-3.83283100	1.13290500	0.19670600
N	3.83281800	-1.13324100	-0.19688100

Dimer of AHTPB

Charge = 0; Multiplicity = 1

C	0.69413800	-0.24075000	0.21522700
H	0.93318900	-1.19171600	-0.27087900
H	0.71187700	-0.40932700	1.30098300
C	4.33762800	1.19344700	-0.06936400
H	4.14453600	2.12109600	0.48643600
H	4.35364900	1.42347500	-1.14621900
C	3.21156500	0.19676900	0.21239200
H	3.24041900	-0.05425700	1.28192700
C	1.81266500	0.75145300	-0.13439800
H	1.78684600	0.96601900	-1.21193200
N	1.61574500	2.00948500	0.64094800
N	1.34813800	3.02187000	-0.01287900
N	3.38515600	-1.02213400	-0.61063300
N	4.23593000	-1.83435700	-0.22572200
N	4.96341200	-2.67873000	0.01327500
N	1.09783100	4.02300700	-0.50347700
C	-0.69464400	0.24027500	-0.21540300

H	-0.93350500	1.19139000	0.27050600
H	-0.71244200	0.40862100	-1.30119300
C	-1.81328700	-0.75169500	0.13456700
H	-1.78748900	-0.96587800	1.21218100
C	-3.21211700	-0.19699800	-0.21241400
H	-3.24103400	0.05331800	-1.28211400
C	-4.33827600	-1.19334000	0.07013000
H	-4.14528900	-2.12142400	-0.48497300
H	-4.35427000	-1.42255600	1.14715900
N	-1.61678400	-2.01006500	-0.64032300
N	-1.34678300	-3.02173500	0.01362300
N	-1.09417400	-4.02225400	0.50430700
N	-3.38541000	1.02248500	0.60980500
N	-4.23618000	1.83454100	0.22453400
N	-4.96359800	2.67886100	-0.01485800
O	-5.54357500	-0.57354800	-0.35312600
H	-6.28991800	-1.11195400	-0.05169700
O	5.54296700	0.57346200	0.35348300
H	6.28927600	1.11207900	0.05234500

Trimer of AHTPB

Charge = 0; Multiplicity = 1

C	-1.90057500	0.48756900	-0.17326300
H	-1.80746300	1.45402400	0.33223300
H	-1.89887700	0.67549800	-1.25630200
C	1.90080400	-0.48742900	0.17354400
H	1.80757800	-1.45417300	-0.33136900
H	1.89915200	-0.67471800	1.25669600
C	0.66691400	0.35514900	-0.17711600
H	0.66411600	0.56631600	-1.25546300
C	-0.66665000	-0.35513100	0.17700200
H	-0.66373600	-0.56661000	1.25528700
N	-0.72709300	-1.62792500	-0.59584500
N	-0.70394100	-2.67295100	0.06200900
N	0.72745400	1.62814600	0.59536600
N	0.70254700	2.67301700	-0.06267300
N	0.68968200	3.70211100	-0.55823800
N	-0.69256400	-3.70215200	0.55738800
C	-3.21785000	-0.17963300	0.23467700
H	-3.32509900	-1.14145300	-0.27522900
H	-3.21687500	-0.37535100	1.31610100
C	3.21808300	0.17946700	-0.23487300
H	3.21709800	0.37440800	-1.31643800
H	3.32531300	1.14165700	0.27434000
C	4.45353100	-0.66735300	0.09845600
H	4.44937700	-0.91475300	1.16924200
C	5.76956700	0.07792700	-0.21839500
H	5.76819500	0.36877800	-1.27813400
C	-4.45330700	0.66741800	-0.09805700
H	-4.44915000	0.91557400	-1.16866900
C	-5.76933600	-0.07809700	0.21826900
H	-5.76800600	-0.36959800	1.27783000
C	7.01837800	-0.76873500	0.03664000
H	7.06465400	-1.02965800	1.10544600
H	6.95460700	-1.69555600	-0.55008500

C	-7.01814800	0.76870300	-0.03630300
H	-6.95440100	1.69516900	0.55098200
H	-7.06438900	1.03026600	-1.10495300
N	5.77864800	1.27817500	0.64927800
N	6.51208900	2.21117600	0.29791900
N	7.11941800	3.15370000	0.09290000
N	4.40976400	-1.91629900	-0.71475000
N	4.45874500	-2.98113900	-0.09120300
N	4.49604100	-4.02621100	0.36893900
N	-4.40957800	1.91577400	0.71603700
N	-4.45830300	2.98106600	0.09323800
N	-4.49529600	4.02648100	-0.36614800
N	-5.77832700	-1.27781300	-0.65013200
N	-6.51185900	-2.21100600	-0.29946300
N	-7.11921600	-3.15365600	-0.09511600
O	-8.12955800	-0.02072400	0.35986800
H	-8.94105100	0.41789800	0.06509700
O	8.12977400	0.02045000	-0.36004400
H	8.94128500	-0.41810900	-0.06522800

Tetramer of AHTPB

Charge = 0; Multiplicity = 1

C	-4.47813000	-0.51412100	0.15133800
H	-4.42247700	-1.47168600	-0.37609000
H	-4.47824000	-0.72627100	1.22989400
C	-0.65084800	0.35077600	-0.20035100
H	-0.71223800	1.31974300	0.30394200
H	-0.65256400	0.53745200	-1.28360700
C	-1.90531500	-0.45740700	0.15604100
H	-1.90828000	-0.67149600	1.23388100
C	-3.21878500	0.29560400	-0.18706000
H	-3.21028500	0.52366900	-1.26191600
N	-3.23909400	1.55748900	0.60586400
N	-3.19560000	2.61166500	-0.03636400
N	-1.87548200	-1.72918600	-0.61984200
N	-2.03495500	-2.77083400	0.02514200
N	-2.16645000	-3.79702700	0.50891800
N	-3.16245900	3.64759900	-0.51637700
C	-5.77429400	0.20571500	-0.23483700
H	-5.84677500	1.15876800	0.29683800
H	-5.77153100	0.42546400	-1.31165800
C	0.65128200	-0.35087300	0.20046000
H	0.65299300	-0.53757600	1.28371100
H	0.71265600	-1.31983200	-0.30385600
C	1.90573100	0.45735100	-0.15591600
H	1.90867500	0.67146600	-1.23375000
C	3.21924500	-0.29559800	0.18717400
H	3.21077800	-0.52364200	1.26203500
C	-7.03566100	-0.60699700	0.08536100
H	-7.03573900	-0.87761100	1.15057800
C	-8.32754300	0.18808900	-0.21033400
H	-8.32188800	0.49690500	-1.26496000
C	4.47854800	0.51416900	-0.15126500
H	4.47867000	0.72619900	-1.22984400
H	4.42281500	1.47178300	0.37606300

C	-9.60304300	-0.62005200	0.03762000
H	-9.57364500	-1.53943500	-0.56346000
H	-9.65341800	-0.89567100	1.10250700
N	3.23972200	-1.55749800	-0.60571900
N	3.19471400	-2.61164600	0.03645300
N	3.16006400	-3.64755900	0.51640400
N	1.87582600	1.72911000	0.62000200
N	2.03520700	2.77078800	-0.02495900
N	2.16651500	3.79700800	-0.50872700
N	-7.03296700	-1.83862700	-0.75475200
N	-7.14815100	-2.91309600	-0.15668300
N	-7.24680500	-3.96475900	0.27852800
N	-8.29143400	1.37280900	0.67777200
N	-8.99624200	2.33519100	0.34743100
N	-9.57359600	3.30042300	0.16262500
O	-10.68888300	0.21194200	-0.34170800
H	-11.51333000	-0.20236000	-0.04767300
C	5.77473200	-0.20557300	0.23502000
H	5.84710100	-1.15881900	-0.29632300
H	5.77207000	-0.42495200	1.31191600
C	7.03611600	0.60694900	-0.08561500
H	7.03618800	0.87703100	-1.15096600
C	8.32798600	-0.18799300	0.21047600
H	8.32241900	-0.49610800	1.26530700
C	9.60346600	0.61997600	-0.03812200
H	9.65378500	0.89482200	-1.10321100
H	9.57405200	1.53979100	0.56229100
O	10.68933800	-0.21172900	0.34175200
H	11.51376300	0.20236100	0.04735400
N	7.03368100	1.83900600	0.75388600
N	7.14676200	2.91328100	0.15507000
N	7.24371100	3.96481000	-0.28084900
N	8.29177300	-1.37329900	-0.67684000
N	8.99668800	-2.33543600	-0.34601600
N	9.57426800	-3.30046700	-0.16086600

Pentamer of AHTPB

Charge = 0; Multiplicity = 1

C	-7.05020100	0.51036300	-0.13977800
H	-7.01051500	1.46138300	0.40074100
H	-7.05026000	0.73718100	-1.21534400
C	-3.21259100	-0.30729700	0.21113300
H	-3.26094800	-1.27148500	-0.30333500
H	-3.21389900	-0.50530900	1.29238800
C	-4.47630000	0.48891200	-0.13896400
H	-4.47933400	0.71586900	-1.21420000
C	-5.78044600	-0.28609200	0.19142300
H	-5.77123000	-0.52777900	1.26328900
N	-5.78126200	-1.53789600	-0.61765000
N	-5.72873200	-2.59957000	0.01148100
N	-4.46237200	1.75141800	0.65204400
N	-4.66174900	2.79645100	0.02354400
N	-4.82943500	3.82469900	-0.44422500
N	-5.68578100	-3.64099700	0.47862700
C	-8.33703700	-0.23319400	0.23255500

H	-8.39362400	-1.18043600	-0.31120600
H	-8.33490800	-0.46633500	1.30656500
C	-1.91832400	0.41440100	-0.17994100
H	-1.91652500	0.61069300	-1.26147400
H	-1.87316100	1.37972800	0.33305600
C	-0.65512900	-0.38180500	0.17345500
H	-0.64886900	-0.59737900	1.25096200
C	0.65271100	0.38133700	-0.17193100
H	0.64652000	0.59657000	-1.24950600
C	-9.60902900	0.56477300	-0.08232400
H	-9.60957800	0.84791600	-1.14429800
C	-10.89015100	-0.25250500	0.19992900
H	-10.88425800	-0.57115600	1.25162000
C	1.91594300	-0.41466500	0.18181200
H	1.91444500	-0.60994700	1.26352600
H	1.87065200	-1.38047500	-0.33026500
C	-12.17650900	0.53887900	-0.04602700
H	-12.16335100	1.45322800	0.56329200
H	-12.22664100	0.82319900	-1.10862600
N	0.67115600	1.65249900	0.60564500
N	0.50438300	2.69363100	-0.03849500
N	0.36490800	3.71910700	-0.52145100
N	-0.67376100	-1.65271800	-0.60451000
N	-0.50680000	-2.69404900	0.03926700
N	-0.36761200	-3.71969200	0.52194400
N	-9.62610600	1.78631800	0.77211800
N	-9.76626300	2.86513700	0.18727000
N	-9.88845300	3.91956900	-0.23501900
N	-10.83273800	-1.42809900	-0.69915200
N	-11.52465000	-2.40381900	-0.38080900
N	-12.08845400	-3.37911800	-0.20743600
O	-13.25140100	-0.31234700	0.32148400
H	-14.08069600	0.09207300	0.02730900
C	3.21009700	0.30664600	-0.21033800
H	3.25874400	1.27133200	0.30316000
H	3.21108200	0.50359100	-1.29179000
C	4.47394700	-0.48912300	0.14011100
H	4.47709700	-0.71553800	1.21546400
C	5.77781400	0.28610000	-0.19073500
H	5.76792700	0.52824600	-1.26248800
C	7.04787200	-0.51025500	0.13947000
H	7.04828100	-0.73811700	1.21481000
H	7.00861000	-1.46079400	-0.40192200
N	4.45995500	-1.75205800	-0.65020900
N	4.66230900	-2.79646900	-0.02164900
N	4.83209000	-3.82426700	0.44636300
N	5.77834000	1.53765200	0.61884600
N	5.73076600	2.59962000	-0.01016200
N	5.69270200	3.64124100	-0.47731400
C	8.33449700	0.23390300	-0.23235600
H	8.39192700	1.17989300	0.31348900
H	8.33150600	0.46948000	-1.30584200
C	9.60642800	-0.56519800	0.07948300
H	9.60708400	-0.85206900	1.14047000
C	10.88748500	0.25336400	-0.19993300

H	10.88040400	0.57775200	-1.24986200
C	12.17433100	-0.53904400	0.04029500
H	12.22539100	-0.82986100	1.10110100
H	12.16140900	-1.44968300	-0.57460000
O	13.24854600	0.31487400	-0.32279000
H	14.07844600	-0.09223600	-0.03405500
N	9.62132200	-1.78373800	-0.77919200
N	9.77984700	-2.86317600	-0.20016700
N	9.91746300	-3.91784200	0.21671100
N	10.83102700	1.42404100	0.70562500
N	11.52216500	2.40170500	0.39157100
N	12.08554600	3.37803100	0.22266600

PBC-HTPB

6	0.549053	0.545983	-0.010446
1	0.229444	1.364462	0.651115
1	0.623164	0.971218	-1.020237
6	4.336234	-0.522512	0.100155
1	4.655506	-1.341365	-0.561169
1	4.262404	-0.947564	1.110068
6	2.991864	-0.006610	-0.334940
1	2.937359	0.380918	-1.355380
6	1.893428	0.030052	0.424919
1	1.947614	-0.357322	1.445420
6	-0.549043	-0.545990	0.010420
1	-0.229433	-1.364469	-0.651142
1	-0.623154	-0.971224	1.020211
6	-1.893417	-0.030059	-0.424947
1	-1.947606	0.357299	-1.445454
6	-2.991849	0.006623	0.334917
1	-2.937343	-0.380889	1.355363
6	-4.336218	0.522526	-0.100180
1	-4.655488	1.341381	0.561142
1	-4.262388	0.947574	-1.110095
-2	9.770822	0.046579	0.178874

PBC-GAP

6	1.446793	0.572173	0.009696
6	2.591479	-0.437404	0.106061
1	2.391133	-1.253466	-0.600790
1	2.630369	-0.853823	1.122806
8	0.264503	-0.178973	0.230279
6	-0.949225	0.478216	-0.095498
1	-1.172765	1.290187	0.609201
1	-0.911469	0.894781	-1.112238
6	-2.072318	-0.556135	-0.007571
1	-2.075953	-0.980681	1.009761
6	-1.870764	-1.722856	-0.978835
1	-0.902256	-2.185725	-0.756802
1	-2.652081	-2.480152	-0.832696
8	-3.268701	0.168363	-0.240653
7	-1.915398	-1.213707	-2.367692
7	-1.509669	-1.995213	-3.232796
7	-1.161098	-2.622356	-4.122139
6	1.613537	1.740870	0.985066

1	2.573818	2.225300	0.773362
1	0.817432	2.481403	0.832907
7	1.566799	1.227839	2.372420
7	1.944194	2.017176	3.243225
7	2.267371	2.650949	4.137441
1	1.443374	0.998685	-1.006796
-2	7.061946	0.077767	0.030754

PBC-AHTPB

6	0.640511	0.420820	0.000000
1	0.663012	1.043625	0.899086
1	0.642811	1.091371	-0.870925
6	4.488646	-0.420232	-0.000989
1	4.467510	-1.043806	-0.899593
1	4.484027	-1.090087	0.870456
6	3.211630	0.429787	0.030889
1	3.208406	1.116588	-0.826880
6	1.918018	-0.428264	-0.035138
1	1.922415	-1.116928	0.821131
7	1.927551	-1.195568	-1.312434
7	2.145673	-2.408812	-1.224126
7	3.201177	1.199906	1.306460
7	2.984180	2.413106	1.214882
7	2.798186	3.538909	1.259348
7	2.332617	-3.534326	-1.271805
6	-0.640515	-0.420816	0.000027
1	-0.663004	-1.043636	-0.899048
1	-0.642824	-1.091352	0.870963
6	-1.918025	0.428266	0.035130
1	-1.922418	1.116901	-0.821162
6	-3.211634	-0.429790	-0.030877
1	-3.208416	-1.116559	0.826918
6	-4.488650	0.420229	0.000960
1	-4.467522	1.043826	0.899548
1	-4.484017	1.090061	-0.870503
7	-1.927584	1.195612	1.312402
7	-2.145643	2.408861	1.224039
7	-2.332539	3.534387	1.271667
7	-3.201170	-1.199956	-1.306420
7	-2.984194	-2.413158	-1.214793
7	-2.798216	-3.538965	-1.259214
-2	10.259060	0.000000	0.000000