Supplementary information for

The effect of π-stacking, h-bonding, and electrostatic interactions on the ionization energies of nucleic acid bases: adenine-adenine, thymine-thymine and adenine-thymine dimers.

Ksenia B. Bravaya[a], Oleg Kostko[b], Musahid Ahmed[b], and Anna I. Krylov[a]

[a] Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0482, USA

[b] Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

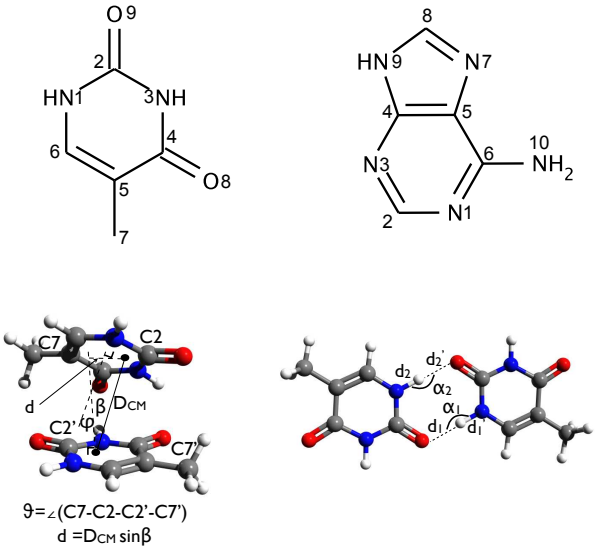

FIG. 1: Definitions of the main parameters characterizing geometries of stacked and h-bonded NAB dimers. For the stacked dimers, these parameters are: distance between the centers of mass (COM) of the fragments (D_{CM}), tilt angle between the planes of the bases (φ), the relative twist of the fragments (θ), and the horizontal displacement of the COM (d). For the h-bonded dimers, the most important structural parameters are the distances between the atoms participating in h-bonding (d and d') and the corresponding angles (α).

TABLE I: Optimized intermolecular structural parameters (see Fig. 1) for optimized stacked NAB dimers[a].

Isomer	Symmetry	State	D_{CM}, Å	φ (tilt)	θ (twist)	d, Å
TT-ST1	C_2	neutral	3.01	8°	37°	0.28
TT-ST2	C_1	neutral	3.38	15°	65°	0.74
TT-ST3	C_1	neutral	3.12	16°	63°	0.15
TT-ST4	C_i	neutral	3.31	0°	180°	1.04
TT-ST5	C_2	neutral	3.49	34°	180°	1.14
TT-ST1	C_1	cation	3.04	0°	41°	0.23
TT-ST3	C_1	cation	3.52	16°	69°	1.37
AA-ST1	C_1	neutral	3.57	10 °	90°	1.93
AA-ST2	C_1	neutral	3.68	8°	171°	1.73
AA-ST3	C_1	neutral	3.28	1°	2°	1.13
AA-ST4	C_i	neutral	3.19	0°	180°	0.67
AA-ST5	C_1	neutral	3.20	0°	180°	0.17
AA-ST6	C_1	neutral	3.55	12°	20°	1.66
AA-ST1	C_1	cation	3.25	2°	121°	1.03
AT-ST1	C_1	neutral	3.10	7°	28°	0.26
AT-ST2	C_1	neutral	3.07	6°	82°	0.12
AT-ST3	C_1	neutral	3.38	9°	37°	1.57

[a]Geometries of the neutrals and the cations were optimized with B3LYP-D/6-31+G(d,p) and ωB97X-D/6-31+G(d,p), respectively.

TABLE II: Optimized intermolecular structural parameters (see Fig. 1) for the neutral and ionized h-bonded NAB dimers.[a]

Isomer	Symm	State	d_1/d_1', Å	α_1	d_2/d_2', Å	α_2
TT-HB1	C_{2h}	neutral	1.767/1.031 (O8···H/H−N5)	178	1.031/1.767 (N5−H/H···O8)	178
TT-HB1 (TS)[b,c]	C_{2h}	cation	1.704/1.037 (O8···H/H−N5)	174	1.037/1.704 (N5−H/H···O8)	174
TT-HB1 (HT)[d]	C_s	cation	1.027/1.608 (O8−H/H···N5)	174	1.033/1.745 (N5−H/H···O8)	174
TT-HB2	C_s	neutral	1.764/1.030 (O7···H/H−N5)	175	1.034/1.814 (N3−H/H···O8)	173
TT-HB2 (HT)[d]	C_s	cation	1.022/1.629 (O7−H/H···N5)	172	1.037/1.756 (N3−H/H···O8)	173
TT-HB3	C_s	neutral	1.779/1.029 (O8···H/H−N5)	175	1.033/1.825 (N3−H/H···O8)	172
TT-HB3 (HT)[d]	C_s	cation	1.039/1.567 (O8−H/H···N5))	173	1.034/1.787 (N3−H/H···O8)	172
AA-HB1	C_{2h}	neutral	1.851/1.037 (N3···H/H−N9)	167	1.037/1.851 (N9−H/H···N3)	167
AA-HB1[b]	C_{2h}	cation	1.854/1.037 (N3···H/H−N9)	166	1.037/1.854 (N9−H/H···N3)	166
AA-HB1 (HT)[d]	C_s	cation	1.045/1.793 (N3−H/H···N9)	164	1.034/1.888 (N9−H/H···N3)	167
AT-HB1	C_1	neutral	1.840/1.038 (N3(A)···H/H−N5(T))	178	1.028/1.801 (N9(A)−H/H···O8(T))	164
AT-HB1[b]	C_1	cation	2.197/1.016 (N3(A)···H/H−N5(T))	170	1.083/1.485 (N9(A)−H/H···O8(T))	176
AT-HB1 (HT)[d]	C_s	cation	1.039/1.866 (N3(A)−H/H···N5(T))	176	1.019/1.904 (N9(A)−H/H···O8(T))	149
AT-HB2	C_1	neutral	1.846/1.039 (N1(A)···H/H−N5(T))	178	1.023/1.845 (N10(A)−H/H···O8(T))	176
AT-HB2	C_1	cation	2.122/1.018 (N1(A)···H/H−N5(T))	167	1.081/1.505 (N10(A)−H/H···O8(T))	176
AT-HB2 (HT)	C_s	cation	1.036/1.913 (N1(A)−H/H···N5(T))	175	1.022/1.827 (N10(A)−H/H···O8(T))	168

[a]Structural parameters for geometries of the neutrals and the cations optimized with ωB97X-D/6-31+G(d,p). [b] Not h-transferred. [c] TS: transition state. [d] HT: h-transferred.

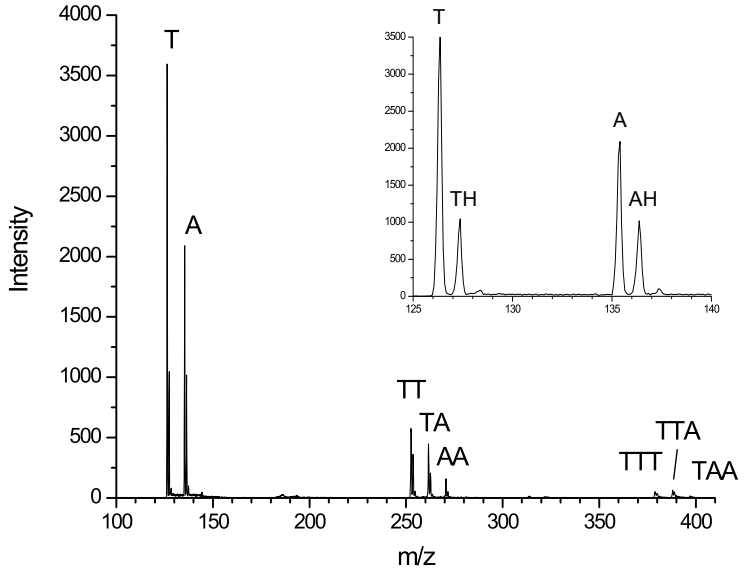

FIG. 2: Mass spectra of the cations formed upon ionization by 10 eV synchrotron radiation

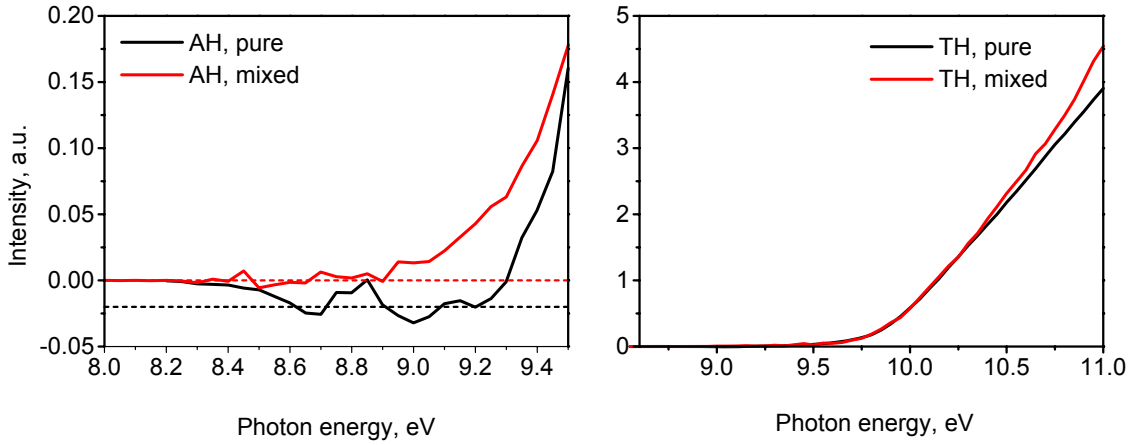

FIG. 3: AH^+ and TH^+ signal dependence on the radiation wavelength for the two types of experimental setup: pure molecular beam (only A or only T in the gas phase) and mixed molecular beam (both A and T are present in the gas phase)

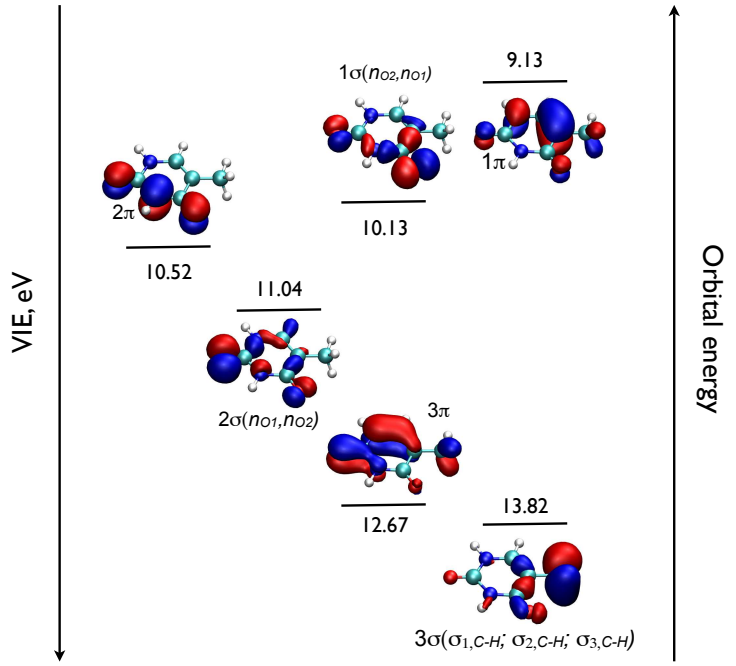

FIG. 4: VIEs (EOM-IP-CCSD/cc-pVTZ//RI-MP2/cc-pVTZ) and corresponding molecular orbitals for thymine base.

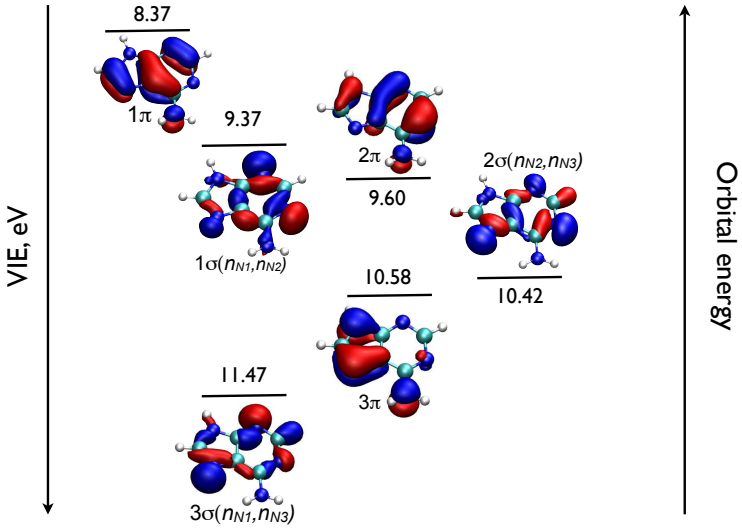

FIG. 5: VIEs (EOM-IP-CCSD/cc-pVTZ//RI-MP2/cc-pVTZ) and corresponding molecular orbitals for adenine base.

TABLE III: Adiabatic and vertical IEs (eV) of the TT, AA, and AT dimers.

	EOM-IP-CCSD/6-311+G(d,p)									
State	TT-HB1	TT-HB2	TT-HB3	TT-ST1	TT-ST3	AA-HB1	AA-ST1	AT-HB1	AT-HB2	AT-ST1
1^{st} AIE	8.23	8.03	8.15	8.41	8.34	7.48	7.57	7.57	7.39	—
1	8.88	8.66	8.68	8.71	8.92	8.23	8.16	8.36	8.30	8.26
2	9.00	9.04	9.10	9.23	9.06	8.26	8.21	8.81	8.64	8.71
3	10.03	9.77	9.78	10.02	9.91	9.36	9.21	9.57	9.59	9.61
4	10.09	10.14	9.89	10.07	10.02	9.43	9.25	9.60	9.79	9.83
5	10.48	10.16	10.17	10.28	10.20	9.49	9.30	9.94	9.81	9.91
6	10.53	10.29	10.28	10.39	10.43	9.49	9.48	10.31	10.17	9.99
7	10.93	10.58	10.65	10.84	—	10.21	10.20	10.43	10.55	—
8	11.27	10.97	11.16	10.87	—	10.28	10.24	10.44	10.56	—
9	—	—	—	—	—	10.29	10.34	10.88	10.85	—
10	—	—	—	—	—	10.35	10.46	11.67	11.60	—
11	—	—	—	—	—	11.07	11.26	—	—	—
12	—	—	—	—	—	—	11.34	—	—	—
	Extrapolated EOM-IP-CCSD/cc-pVTZ (see text)									
1^{st} AIE	8.30	8.12	8.23	8.48	8.41	7.50	7.59	7.60	7.42	—
1	8.95	8.73	8.76	8.78	8.99	8.25	8.18	8.39	8.33	8.28
2	9.07	9.11	9.17	9.30	9.13	8.28	8.23	8.88	8.71	8.89
3	10.13	9.88	9.89	10.12	10.02	9.39	9.25	9.59	9.62	9.32
4	10.19	10.25	9.99	10.17	10.13	9.46	9.29	9.64	9.81	9.51
5	10.59	10.27	10.28	10.39	10.31	9.52	9.31	10.04	9.91	*9.97*
6	10.64	10.40	10.39	10.50	10.54	9.51	9.50	*10.40*	*10.26*	*10.07*
7	11.03	10.67	10.74	10.93	—	10.28	—	10.46	*10.61*	—
8	11.36	11.06	11.25	10.96	—	10.34	—	*10.52*	*10.65*	—
9	—	—	—	—	—	10.33	—	10.97	*10.91*	—
10	—	—	—	—	—	10.39	—	11.72	11.65	—
11	—	—	—	—	—	11.12	—	—	—	

Numbers given in cursive correspond to non-Koopmans ionized states (more than one orbital is significantly involved) or states with delocalized molecular orbitals over the A and T bases. The energy additivity scheme corrections should be considered with caution in these cases. Ionized states 7-12 of AA stacked dimers are strongly multiconfigurational (three or more orbitals are involved) and thus energy additivity correction is not applicable.

TABLE IV: Total NBO charges for each base in the dimer. NBO analysis was performed for IP-CISD/6-31+G(d,p) electron density for the first ionized state.

isomer	fragment 1, charge	fragment 2, charge
TT dimers		
TT-HB1 (geometry of neutral)	T, 0.50	T, 0.50
TT-HB1	0.50	0.50
TT-HB1 (HT)	(T–H)$^{\cdot}$, 0.14	TH^{+}, 0.86
TT-HB2 (geometry of neutral)	T, 0.97	T, 0.03
TT-HB2	(T-H)$^{\cdot}$, 0.13	TH^{+}, 0.87
TT-HB6 (geometry of neutral)	T, 0.97	T, 0.03
TT-HB6	T, 0.89	T, 0.11
TT-HB6 (HT)	(T-H)$^{\cdot}$, 0.15	TH^{+}, 0.85
TT-ST1 (geometry of neutral)	T, 0.50	T, 0.50
TT-ST1	T, 0.50	T, 0.50
TT-ST2 (geometry of neutral)	T, 0.75	T, 0.25
TT-ST2	T, 0.85	T, 0.15
AA dimers		
AA-HB1 (geometry of neutral)	A, 0.50	A, 0.50
AA-HB1	A, 0.50	A, 0.50
AA-HB1 (HT)	(A–H)$^{\cdot}$, 0.10	AH^{+}, 0.90
AA-ST1 (geometry of neutral)	A, 0.53	A, 0.47
AA-ST1	A, 0.61	A, 0.39
AT dimers		
AT-HB1 (geometry of neutral)	A, 0.99	T, 0.01
AT-HB1	A, 0.92	T, 0.08
AT-HB1 (HT)	AH^{+}, 0.93	(T–H)$^{\cdot}$, 0.07

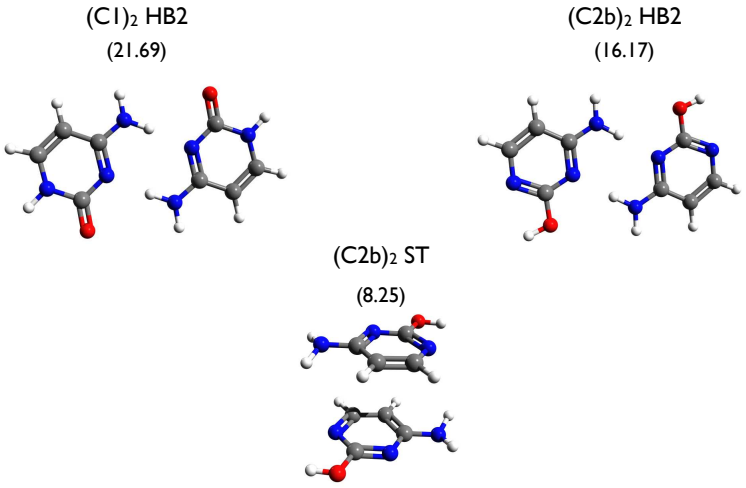

FIG. 6: ωB97X-D/6-31+G(d,p) optimized structures of the CC dimers with equivalent fragments used for DMO-LCFMO analysis. Binding energies computed at the ωB97X-D/6-311++G(2df,2pd)//ωB97X-D/6-31+G(d,p) level of theory are given in parentheses (kcal/mol).

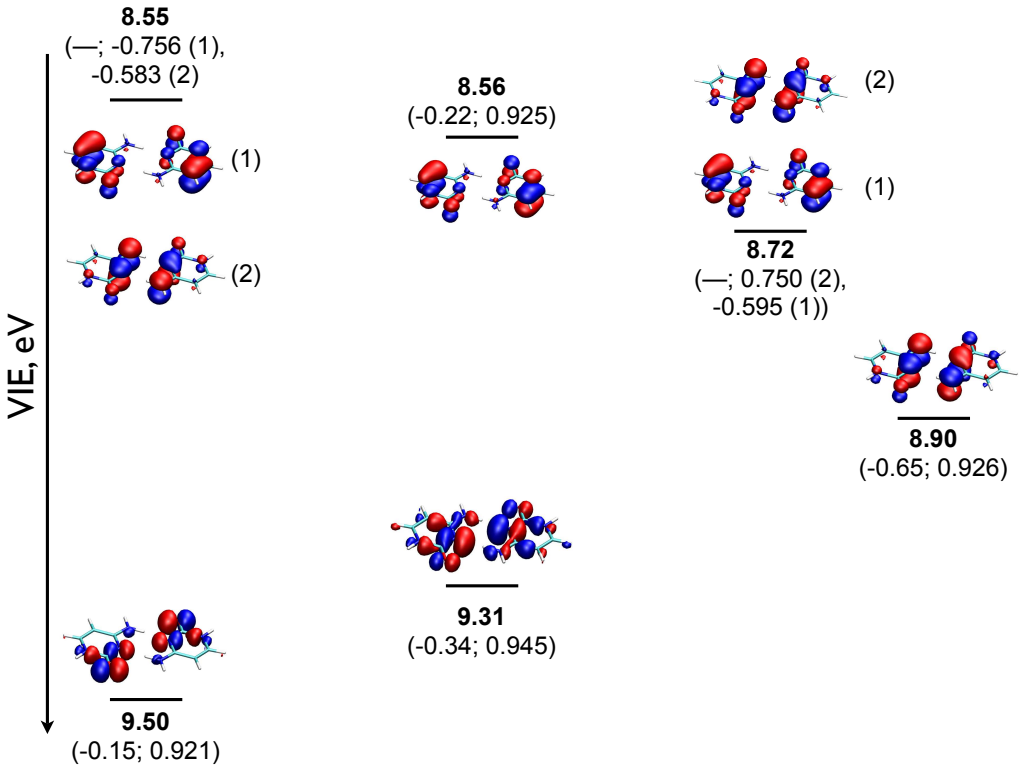

FIG. 7: MOs and respective VIEs (eV, EOM-IP-CCSD/6-311+G(d,p) extrapolated to EOM-IP-CCSD/cc-pVTZ using energy additivity scheme) for the $(C1)_2$-HB2 dimer. Energy difference between the dimer IE and corresponding IE of the monomer (in eV) and leading EOM amplitudes are shown in parenthesis.

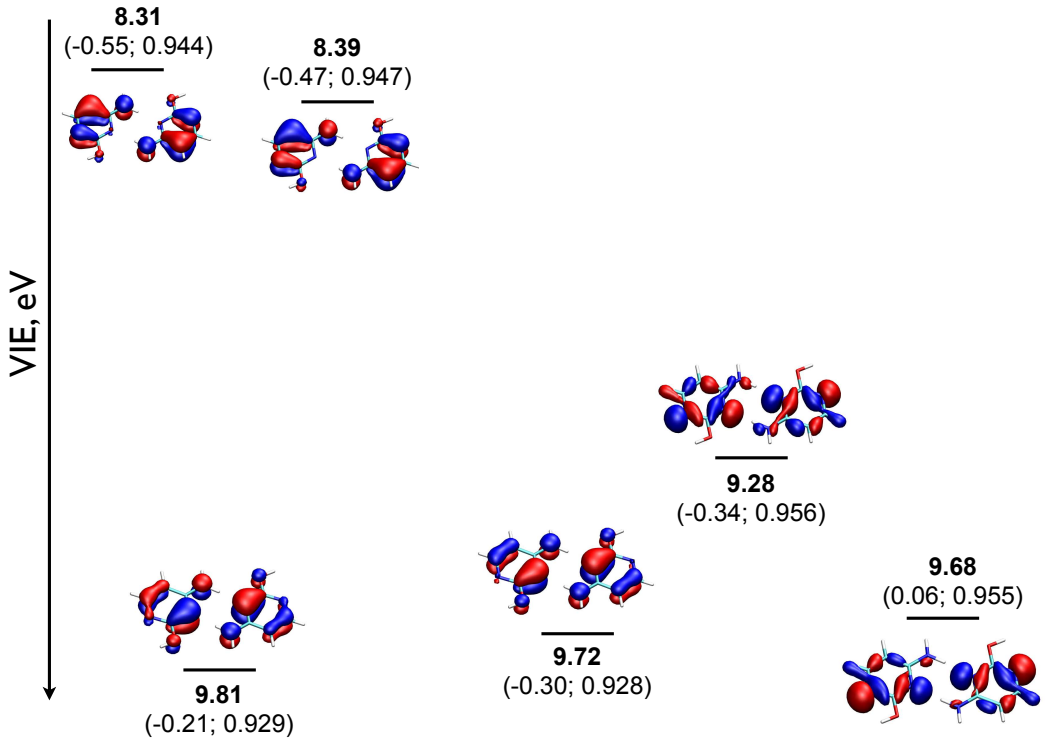

FIG. 8: MOs and respective VIEs (eV, EOM-IP-CCSD/6-311+G(d,p) extrapolated to EOM-IP-CCSD/cc-pVTZ using energy additivity scheme) for the $(C2b)_2$-HB2 dimer. Energy difference between the dimer IE and corresponding IE of the monomer (in eV) and leading EOM amplitudes are shown in parenthesis.

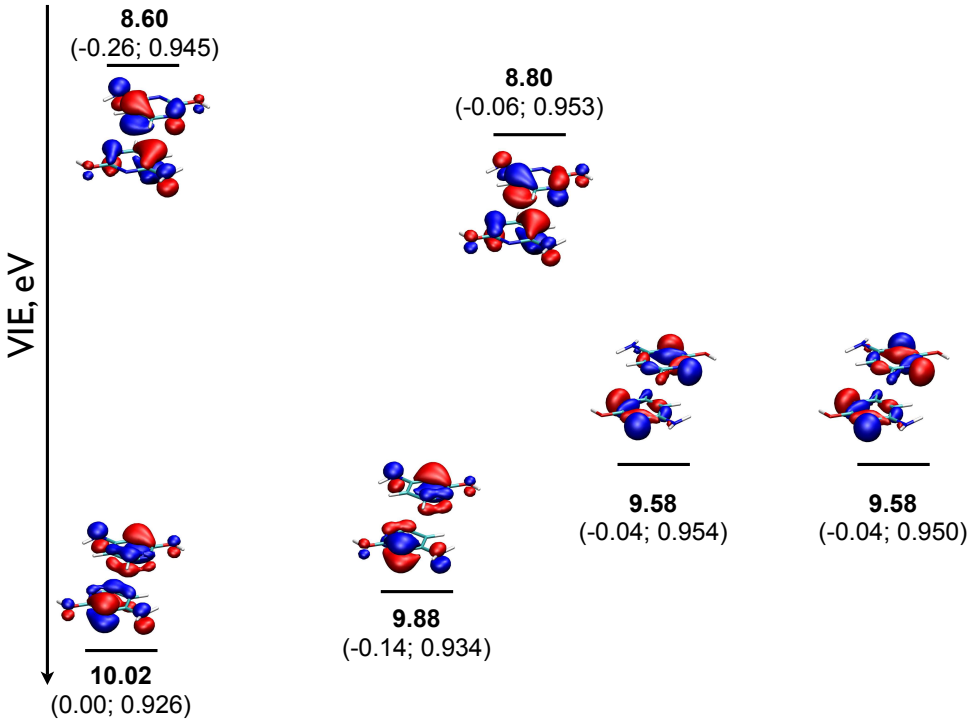

FIG. 9: MOs and respective VIEs (eV, EOM-IP-CCSD/6-311+G(d,p) extrapolated to EOM-IP-CCSD/cc-pVTZ using energy additivity scheme) for the $(C2b)_2$-ST dimer. Energy difference between the dimer IE and corresponding IE of the monomer (in eV) and leading EOM amplitudes are shown in parenthesis.

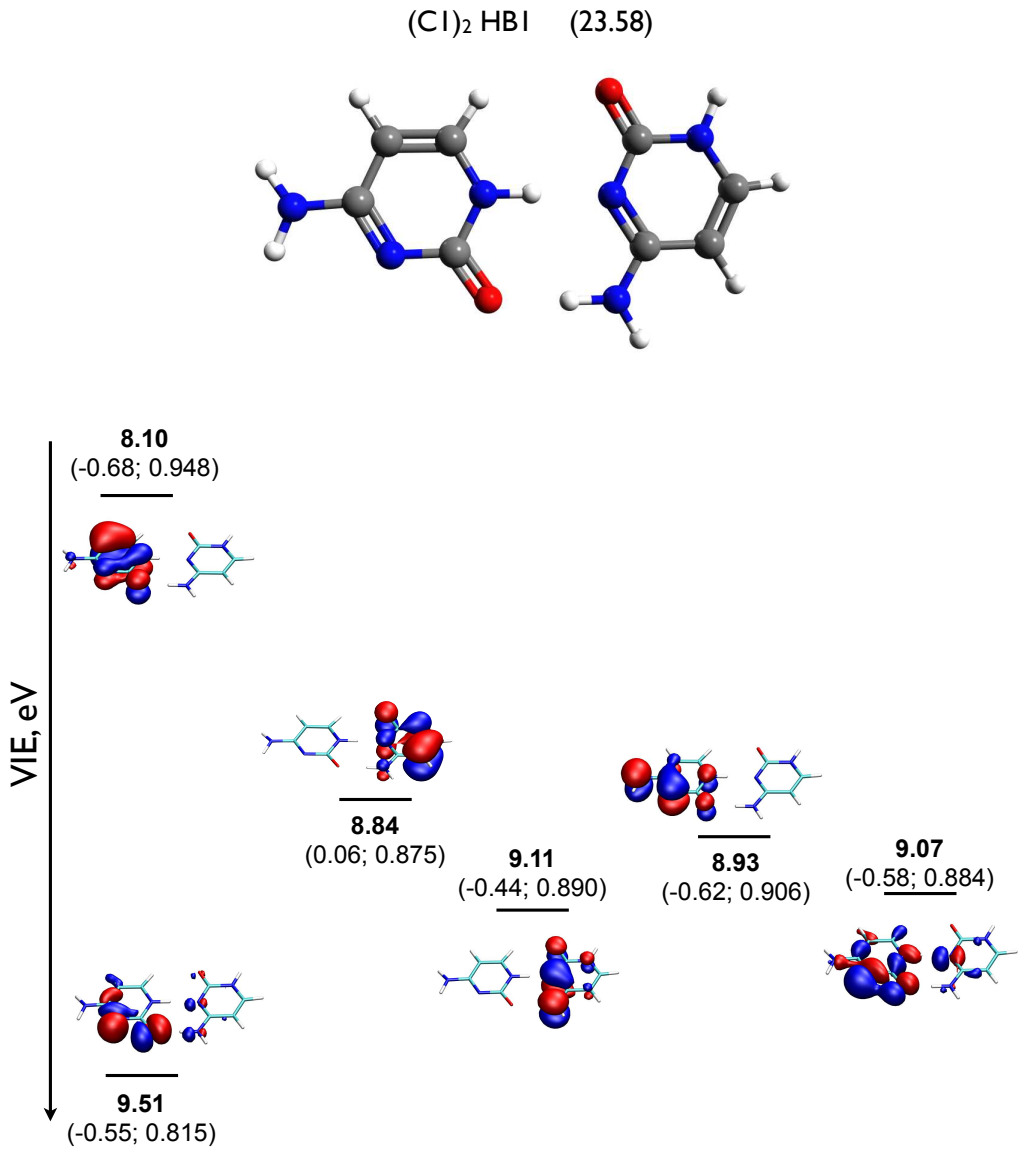

FIG. 10: Structure of the h-bonded cytosine dimer ($(C1)_2$-HB1) used for analysis of the effects of interfragment electrostatic interactions on the ionization energies of the dimers with non-equivalent fragments (upper panel). ωB97X-D/6-311++G(2df,2pd)//ωB97X-D/6-31+G(d,p) binding energy is given in parentheses (kcal/mol). Bottom panel shows MOs and respective VIEs (eV, EOM-IP-CCSD/6-311+G(d,p) extrapolated to EOM-IP-CCSD/cc-pVTZ using energy additivity scheme) for $(C1)_2$-HB1 dimer. Energy difference between the dimer IE and corresponding IE of the monomer (in eV) and leading EOM amplitudes are shown in parenthesis.

Supplementary information for

The effect of π-stacking, h-bonding, and electrostatic interactions on the ionization energies of nucleic acid bases: adenine-adenine, thymine-thymine and adenine-thymine dimers.

Ksenia B. Bravaya[a], Oleg Kostko[b], Musahid Ahmed[b], and Anna I. Krylov[a]

[a] Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0482, USA

[b] Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Equilibrium geometry configurations of NA dimers

A. B3LYP-D/6-31+G(d,p) geometries of neutral dimers

TT-HB1, C_{2h}, E=-908.398833248

H	3.130831	2.438223	0.000000
H	-2.708747	2.322662	0.000000
H	-5.148886	2.638728	0.000000
H	-6.009205	1.347009	0.879542
O	5.350666	1.332647	0.000000
N	3.067800	1.426206	0.000000
O	0.784875	1.608956	0.000000
C	-5.394886	1.572015	0.000000
C	-2.893721	1.253796	0.000000
H	-0.818910	0.915296	0.000000
C	4.290942	0.719485	0.000000
C	1.798611	0.893983	0.000000
H	-6.009205	1.347009	-0.879542
C	-4.147361	0.737321	0.000000
N	-1.755734	0.474501	0.000000
N	1.755734	-0.474501	0.000000

C	4.147361	-0.737321	0.000000
H	6.009205	-1.347009	-0.879542
C	-1.798611	-0.893983	0.000000
C	-4.290942	-0.719485	0.000000
H	0.818910	-0.915296	0.000000
C	2.893721	-1.253796	0.000000
C	5.394886	-1.572015	0.000000
O	-0.784875	-1.608956	0.000000
N	-3.067800	-1.426206	0.000000
O	-5.350666	-1.332647	0.000000
H	6.009205	-1.347009	0.879542
H	5.148886	-2.638728	0.000000
H	2.708747	-2.322662	0.000000
H	-3.130831	-2.438223	0.000000

TT-HB2, C_s, E=-908.393284009

N	2.877413	1.379864	0.000000
H	2.977537	2.388923	0.000000
C	1.585259	0.897137	0.000000
O	0.600640	1.644194	0.000000
N	1.492558	-0.471522	0.000000
H	0.535067	-0.862842	0.000000
C	2.598444	-1.292607	0.000000
H	2.374994	-2.354314	0.000000
C	3.871092	-0.823839	0.000000
C	4.070039	0.626821	0.000000
O	5.155288	1.195860	0.000000
C	5.086209	-1.705297	0.000000
H	4.799766	-2.762102	0.000000
H	5.709098	-1.504229	0.879424
H	5.709098	-1.504229	-0.879424
O	-2.987231	2.758607	0.000000

C	-3.109175	1.546352	0.000000
N	-4.356002	0.921292	0.000000
H	-5.149145	1.547389	0.000000
C	-4.527557	-0.443071	0.000000
H	-5.556976	-0.785773	0.000000
C	-3.479931	-1.303361	0.000000
N	-2.046958	0.652274	0.000000
H	-1.098437	1.071934	0.000000
C	-2.135122	-0.732950	0.000000
O	-1.110193	-1.434571	0.000000
C	-3.628257	-2.797452	0.000000
H	-4.685386	-3.082481	0.000000
H	-3.142548	-3.234880	0.879931
H	-3.142548	-3.234880	-0.879931

TT-HB3, C_s, E=-908.392121031

N	1.964927	0.160029	0.000000
H	1.074973	0.690548	0.000000
C	1.860916	-1.204559	0.000000
O	0.787724	-1.824264	0.000000
N	3.065788	-1.876484	0.000000
H	3.003152	-2.884553	0.000000
C	4.293636	-1.236307	0.000000
H	5.157849	-1.891566	0.000000
C	4.399765	0.110764	0.000000
C	3.162490	0.907594	0.000000
O	3.130960	2.129189	0.000000
C	5.708431	0.844416	0.000000
H	6.550159	0.144180	0.000000
H	5.782540	1.495102	0.878876
H	5.782540	1.495102	-0.878876
O	-0.571392	1.426641	0.000000

C	-1.636235	0.800822	0.000000
N	-1.706068	-0.570091	0.000000
H	-0.804069	-1.071326	0.000000
C	-2.901129	-1.255690	0.000000
H	-2.804332	-2.336309	0.000000
C	-4.109474	-0.640258	0.000000
N	-2.863258	1.431296	0.000000
H	-2.843952	2.445152	0.000000
C	-4.136040	0.823936	0.000000
O	-5.146831	1.516451	0.000000
C	-5.419909	-1.372309	0.000000
H	-5.260178	-2.455539	0.000000
H	-6.014934	-1.099418	-0.879390
H	-6.014934	-1.099418	0.879390

TT-ST1, C_2, E=-908.385439411

H	2.797655	0.051630	-2.792571
H	0.472687	2.550906	-1.715093
C	0.822131	1.868094	-0.949027
H	-0.073004	3.027655	0.521583
C	1.456076	0.709910	-1.248183
N	0.554268	2.254454	0.345532
C	1.826497	-0.180701	-0.146585
C	0.836195	1.467846	1.451326
N	1.542116	0.314350	1.136235
O	0.481268	1.756720	2.583526
O	2.322256	-1.296131	-0.285087
H	1.707480	-0.315012	1.916647
C	1.730335	0.253739	-2.649405
H	1.408120	1.007229	-3.375062
H	1.198582	-0.683312	-2.853381
H	-2.797655	-0.051630	-2.792571

H	-0.472687	-2.550906	-1.715093
C	-0.822131	-1.868094	-0.949027
H	0.073004	-3.027655	0.521583
C	-1.456076	-0.709910	-1.248183
N	-0.554268	-2.254454	0.345532
C	-1.826497	0.180701	-0.146585
C	-0.836195	-1.467846	1.451326
N	-1.542116	-0.314350	1.136235
O	-0.481268	-1.756720	2.583526
O	-2.322256	1.296131	-0.285087
H	-1.707480	0.315012	1.916647
C	-1.730335	-0.253739	-2.649405
H	-1.408120	-1.007229	-3.375062
H	-1.198582	0.683312	-2.853381

TT-ST2, C_1, E=-908.385350082

C	2.308033	-1.339569	-1.768326
C	1.756958	-0.108942	-1.110009
C	0.796269	0.669930	-1.659295
N	0.258417	1.768824	-1.013225
C	0.592121	2.120968	0.280523
N	1.648203	1.388310	0.790458
H	1.936269	1.625970	1.732927
C	2.241485	0.238778	0.228880
O	3.080745	-0.387282	0.864151
O	-0.006591	2.981629	0.917924
H	-0.562759	2.225007	-1.394857
H	0.375190	0.464295	-2.636867
H	1.912756	-1.446078	-2.783307
H	3.402075	-1.299227	-1.807587
H	2.030599	-2.231853	-1.195484
N	-1.936780	-0.870278	-0.864085

H	-2.138861	-1.146549	-1.818326
C	-2.319263	0.412646	-0.515410
O	-2.815236	1.206908	-1.308281
N	-2.055597	0.722894	0.804487
H	-2.177679	1.698257	1.051614
C	-1.283006	-0.082952	1.622681
H	-1.070244	0.334460	2.600342
C	-0.806163	-1.288545	1.233583
C	-1.121685	-1.748720	-0.121232
O	-0.730157	-2.793548	-0.625624
C	0.075829	-2.149126	2.091505
H	0.126228	-1.755569	3.111828
H	-0.301355	-3.176941	2.120711
H	1.093060	-2.185419	1.683487

TT-ST3, C_1**, E=-908.384162157**

C	-0.680221	1.774938	-0.220433
C	-0.909771	1.428567	1.185427
C	-1.687305	0.354917	1.461178
N	-2.291157	-0.398883	0.477311
C	-2.078218	-0.187653	-0.876689
H	-2.686138	-1.300805	0.710897
N	-1.350902	0.958864	-1.147564
O	0.041940	2.687894	-0.606706
O	-2.477344	-0.959153	-1.737834
H	-1.093075	1.085521	-2.121737
H	-1.874649	0.019738	2.475335
C	-0.226996	2.251180	2.237770
H	-0.513311	1.917253	3.240710
H	-0.481919	3.311161	2.128313
H	0.862999	2.178698	2.134214
H	3.557202	0.755276	-1.768558

C	2.178382	-0.009343	-0.312703
C	1.229646	-0.683299	-1.206033
C	2.209109	-0.389927	0.985345
C	3.015807	1.097282	-0.879976
C	0.383529	-1.991315	0.751868
N	1.368320	-1.362854	1.496083
N	0.421519	-1.660194	-0.588812
O	1.090837	-0.439030	-2.397053
O	-0.440978	-2.752638	1.244920
H	1.379151	-1.592362	2.479478
H	2.885548	0.060402	1.703687
H	-0.295345	-2.081241	-1.174661
H	3.732447	1.462516	-0.136944
H	2.366338	1.926515	-1.185291

TT-ST4, C_i, E=-908.3833141180

C	0.00000000	0.00000000	0.00000000
H	-0.78601400	0.04815400	0.75875000
H	0.26030900	-1.05678000	-0.13277900
C	1.20810000	0.78715400	0.41609000
C	1.85340900	0.45893000	1.68899700
O	1.42362100	-0.34175700	2.51488800
N	3.04735500	1.15468300	1.94074500
H	3.53697200	0.91994800	2.79674400
C	3.59014000	2.19907600	1.20697400
O	4.59805500	2.80490800	1.53828000
N	2.86231700	2.49259100	0.06666200
C	1.73056200	1.80127200	-0.31470400
H	1.27870100	2.13663200	-1.24154900
H	3.16115600	3.31054800	-0.44727400
H	-0.40788500	0.38569600	-0.93966100
O	0.85280700	5.16447500	0.23989000

C	0.42301900	4.36378800	1.06578100
N	-0.77092700	3.66803500	0.81403300
H	-1.26054400	3.90277000	-0.04196600
C	-1.31371200	2.62364200	1.54780400
O	-2.32162700	2.01781000	1.21649800
N	-0.58588900	2.33012700	2.68811600
C	0.54586600	3.02144600	3.06948200
C	1.06832800	4.03556400	2.33868800
C	2.27642800	4.82271800	2.75477800
H	3.06244200	4.77456400	1.99602800
H	2.01611900	5.87949800	2.88755700
H	2.68431300	4.43702200	3.69443900
H	0.99772700	2.68608600	3.99632700
H	-0.88472800	1.51217000	3.20205200

TT-ST5, C_2, E=-908.3817421908

C	0.00000000	0.00000000	0.00000000
C	-1.45454300	0.37047600	0.01301500
C	-2.12476900	0.83841300	-1.06607100
N	-3.47941100	1.11249600	-1.03969500
C	-4.28804500	0.88790500	0.06682400
N	-3.57899600	0.46890300	1.17890700
H	-4.13874000	0.21526900	1.98994000
C	-2.20932500	0.16330600	1.25250300
O	-1.73254900	-0.27257300	2.29591100
O	-5.50037800	1.04594900	0.04467500
H	-3.95997900	1.43951300	-1.86557000
H	-1.63462300	1.01734500	-2.01718400
H	0.45974500	0.26984200	-0.95658200
H	0.53382500	0.50647800	0.81157000
H	0.10967700	-1.07960600	0.15772600
N	-3.08179800	-2.72649300	1.17890700

H	-2.52205400	-2.47285900	1.98994000
C	-2.37274900	-3.14549500	0.06682400
O	-1.16041600	-3.30353900	0.04467500
N	-3.18138300	-3.37008600	-1.03969500
H	-2.70081500	-3.69710300	-1.86557000
C	-4.53602500	-3.09600300	-1.06607100
H	-5.02617100	-3.27493500	-2.01718400
C	-5.20625100	-2.62806600	0.01301500
C	-4.45146900	-2.42089600	1.25250300
O	-4.92824500	-1.98501700	2.29591100
C	-6.66079400	-2.25759000	0.00000000
H	-7.12053900	-2.52743200	-0.95658200
H	-7.19461900	-2.76406800	0.81157000
H	-6.77047100	-1.17798400	0.15772600

AA-HB1, C_{2h}, **E=-934.762960408**

H	6.306448	0.877476	0.000000
H	2.349822	3.024994	0.000000
N	3.925667	1.700061	0.000000
C	2.613107	1.970068	0.000000
N	5.636908	0.123873	0.000000
H	5.942501	-0.836834	0.000000
C	4.316045	0.408860	0.000000
H	-1.820123	3.393478	0.000000
N	1.588242	1.107244	0.000000
C	-2.152511	2.363801	0.000000
H	-0.208865	1.373792	0.000000
C	3.333710	-0.602690	0.000000
C	2.000326	-0.177295	0.000000
N	-1.250714	1.323859	0.000000
N	-3.413164	1.981441	0.000000
N	3.413164	-1.981441	0.000000

C	-2.000326	0.177295	0.000000
N	1.250714	-1.323859	0.000000
C	-3.333710	0.602690	0.000000
C	2.152511	-2.363801	0.000000
H	-5.942501	0.836834	0.000000
H	0.208865	-1.373792	0.000000
N	-1.588242	-1.107244	0.000000
C	-4.316045	-0.408860	0.000000
H	1.820123	-3.393478	0.000000
N	-5.636908	-0.123873	0.000000
C	-2.613107	-1.970068	0.000000
H	-6.306448	-0.877476	0.000000
N	-3.925667	-1.700061	0.000000
H	-2.349822	-3.024994	0.000000

AA-ST1, C_1, E=-934.745724222

H	-2.834372	-2.827774	-0.095099
C	-2.421533	-1.857494	0.171482
H	0.442668	-2.516571	-2.043933
N	-1.323100	-1.891033	0.943320
N	-3.065728	-0.790733	-0.316879
H	-0.928707	-0.561356	-2.960494
N	0.614423	-1.544828	-1.830351
C	-0.107607	-0.452301	-2.265103
C	-0.761276	-0.726192	1.321946
H	0.839972	-1.641867	2.144645
C	-2.482886	0.349426	0.075717
N	2.475946	-1.759533	-0.259924
C	1.554458	-1.071273	-0.946647
N	0.344779	-0.761835	2.105687
C	-1.354948	0.480375	0.893590
H	-3.595994	1.913570	-0.847909

N	-2.829181	1.640046	-0.251020
N	0.295696	0.680578	-1.739903
C	1.338274	0.311867	-0.906540
H	0.898484	0.078440	2.187841
C	3.209461	-0.955007	0.515907
H	3.992645	-1.434327	1.098545
N	-1.009173	1.811920	1.058031
C	-1.910075	2.463900	0.360341
N	3.094086	0.374890	0.687700
C	2.152899	1.037196	-0.012626
H	-1.960350	3.539627	0.255504
H	1.089813	2.746140	-0.001399
N	2.018292	2.379496	0.164606
H	2.508140	2.761539	0.962679

AA-ST2, C_1, E=-934.745542008

H	-2.393719	-2.762302	1.792691
H	1.387247	-1.842367	2.229015
H	0.243261	-0.597765	2.555018
N	1.150560	-0.860518	2.194026
H	-3.631451	-1.599782	2.136191
N	-2.729137	-1.811534	1.734603
N	-0.360486	-2.498214	-0.085885
H	1.346878	-2.863576	-1.300795
C	0.494472	-2.248758	-1.049970
C	-2.339565	-1.065488	0.661495
C	1.605858	-0.172708	1.117732
C	-1.231256	-1.422439	-0.127583
N	2.627786	-0.674497	0.396300
N	-3.006910	0.064955	0.374687
C	1.046010	1.060753	0.727103
N	0.224091	-1.082522	-1.736415

N	0.010430	1.814584	1.244629
C	-0.885626	-0.524757	-1.144577
C	3.034731	-0.000962	-0.692333
H	3.862304	-0.450528	-1.236979
H	0.821845	-0.627363	-2.412950
C	-2.563032	0.826522	-0.639317
C	1.557224	1.629650	-0.444546
N	-1.515135	0.617940	-1.445397
C	-0.100595	2.816413	0.405127
N	2.544774	1.134849	-1.206077
H	-0.823677	3.616928	0.482916
H	-3.135693	1.731876	-0.826114
N	0.811133	2.768747	-0.628757
H	0.865639	3.391309	-1.421467

AA-ST3, C_1, E=-934.744335569

H	4.075031	0.647872	1.330228
H	2.757459	2.492414	0.147877
C	3.251230	0.467339	0.652427
N	2.606285	1.503610	0.012627
H	-1.359120	2.999406	0.276565
N	2.768686	-0.715351	0.345408
C	1.614655	0.940105	-0.756573
N	-0.125290	1.028171	1.829232
H	1.274685	-0.021093	3.041608
N	-2.180164	2.459796	0.041940
H	-2.738138	2.786456	-0.734548
C	1.744532	-0.436973	-0.544074
N	0.704596	1.547657	-1.526932
C	0.431049	-0.031583	2.366296
C	-1.135322	0.510174	1.034566
C	-2.090277	1.110739	0.189670

C	-0.109271	0.659556	-2.111955
C	0.819131	-1.257566	-1.219903
H	1.422480	-3.019567	-0.398788
N	-0.156049	-1.215502	1.973181
H	-0.890771	1.071209	-2.744502
N	-0.102032	-0.679131	-2.008261
N	0.831178	-2.611071	-1.106916
C	-1.171946	-0.886634	1.104491
N	-2.951924	0.321564	-0.475597
H	0.127664	-2.148866	2.230644
H	-0.018121	-3.097234	-1.358414
C	-2.859450	-1.009530	-0.317226
N	-2.006967	-1.701591	0.448011
H	-3.570676	-1.597313	-0.891523

AA-ST4, C_i, E=-934.7441766194

C	0.00000000	0.00000000	0.00000000
N	-0.99122900	-0.08754300	0.96164600
C	-2.10471700	-0.09108900	0.26929800
H	-3.10073400	-0.13883500	0.68810500
N	-1.90148000	-0.02268000	-1.09412300
H	-2.60618700	0.00523700	-1.81558100
C	-0.54164800	0.04563600	-1.28855800
N	0.13647600	0.14406100	-2.43969200
C	1.45602100	0.19335200	-2.22733000
H	2.07889000	0.28724000	-3.11202200
N	2.11749200	0.16123700	-1.05584600
C	1.40505900	0.06718400	0.08108700
N	2.05745600	0.01828900	1.27185300
H	1.52826000	0.24846900	2.10093800
H	3.04274900	0.23623300	1.26378500
C	0.85963400	3.23613400	-1.30534000

N	1.85086300	3.32367700	-2.26698600
C	2.96435100	3.32722300	-1.57463800
H	3.96036800	3.37496900	-1.99344500
N	2.76111400	3.25881400	-0.21121700
H	3.46582100	3.23089700	0.51024100
C	1.40128200	3.19049800	-0.01678200
N	0.72315800	3.09207300	1.13435200
C	-0.59638700	3.04278200	0.92199000
H	-1.21925600	2.94889400	1.80668200
N	-1.25785800	3.07489700	-0.24949400
C	-0.54542500	3.16895000	-1.38642700
N	-1.19782200	3.21784500	-2.57719300
H	-0.66862600	2.98766500	-3.40627800
H	-2.18311500	2.99990100	-2.56912500

AA-ST5, C_1, E=-934.743139637

H	2.676941	-1.521056	1.420151
N	2.450379	-0.834534	0.715989
N	1.121928	0.730566	2.044023
H	3.324305	-1.697197	-1.049342
C	1.647217	0.264725	0.904926
C	2.722487	-0.900250	-0.634723
H	-0.010184	-3.483421	1.624362
H	-0.084804	2.262040	2.708291
H	-0.885409	-2.243594	2.465818
N	-0.367973	-2.539913	1.650718
C	0.383462	1.822981	1.831685
C	1.490244	0.810314	-0.375057
N	2.177943	0.073927	-1.324425
C	-0.669223	-1.951631	0.459594
N	0.129503	2.449613	0.666738
C	0.672069	1.953582	-0.459054

N	-0.128508	-2.449019	-0.666396
N	-2.175508	-0.072168	1.324858
C	-1.488250	-0.808928	0.375478
H	0.891925	2.248855	-2.464591
N	0.373338	2.543743	-1.649746
C	-0.385012	-1.824203	-1.831863
H	0.081932	-2.264333	-2.708641
H	0.013177	3.486303	-1.622800
C	-2.722836	0.900057	0.634607
C	-1.648236	-0.265514	-0.905046
H	-3.325247	1.696654	1.049041
N	-1.124677	-0.732715	-2.044426
N	-2.452593	0.832916	-0.716422
H	-2.683879	1.516618	-1.421792

AA-ST6, C_1, E=-934.742859804

N	-0.183799	1.829708	-1.184568
C	-0.844656	2.526629	-0.245362
H	-0.477450	3.534277	-0.068119
N	-1.886771	2.140648	0.499877
C	-2.251687	0.887748	0.208044
C	-0.574897	0.571564	-1.457419
N	0.084554	-0.126781	-2.419417
H	0.009559	-1.134559	-2.364647
H	1.006606	0.226244	-2.648044
N	-3.265788	0.142522	0.769585
H	-3.914118	0.467624	1.472220
C	-3.254700	-1.084935	0.134474
H	-3.972463	-1.855924	0.382891
N	-2.311892	-1.191443	-0.771613
C	-1.670953	0.037852	-0.742159

N	1.158120	-2.166443	-0.341758
C	0.202789	-2.523909	0.484080
H	-0.414440	-3.404386	0.377101
N	0.021610	-1.640699	1.526731
H	-0.683787	-1.685034	2.247023
C	0.925056	-0.617049	1.342399
N	1.108936	0.482046	2.080283
C	2.076515	1.256685	1.574879
H	2.294246	2.169211	2.123419
N	2.817595	1.053722	0.470692
C	2.589837	-0.049422	-0.257000
N	3.260624	-0.217030	-1.439299
H	3.317303	-1.158562	-1.803124
H	4.068080	0.376222	-1.576363
C	1.623055	-0.970682	0.181987

AT-HB1, C_1, E=-921.580283264

H	5.990680	0.261936	0.007501
H	5.818471	2.006005	0.007529
N	5.408496	1.085033	0.009942
C	4.063858	0.957723	0.006878
N	3.916164	-1.595541	0.005675
N	3.302013	2.071889	0.005763
C	3.430653	-0.302343	0.005408
C	2.827886	-2.337474	0.003632
H	2.815707	-3.419133	0.003179
C	1.969674	1.936226	0.003504
C	2.031727	-0.293949	0.003158
H	1.402969	2.864153	0.002647
N	1.658956	-1.610112	0.002120
N	1.250614	0.805001	0.002169
H	0.680973	-1.938493	-0.000302

H	-0.528210	0.451838	0.000450
O	-1.091749	-2.045098	-0.004659
N	-1.543977	0.213925	0.004308
C	-1.902639	-1.109138	0.002315
H	-2.051103	2.230064	0.012779
C	-2.474534	1.230957	0.012025
H	-5.480364	2.043824	0.907311
N	-3.263880	-1.330159	0.008941
H	-3.558801	-2.300286	0.007696
C	-3.814118	1.020988	0.018347
C	-4.290346	-0.362473	0.017006
H	-4.344720	3.103667	0.029706
C	-4.832907	2.123496	0.026392
O	-5.464084	-0.713025	0.022360
H	-5.485207	2.052483	-0.851747

AT-HB2, C_1, **E=-921.576139949**

H	5.595897	-1.924127	0.827561
H	3.793678	2.492637	0.028747
O	5.653147	0.849723	-0.005547
N	3.471786	1.531330	0.014108
C	4.468650	0.534786	-0.006409
H	-0.503353	2.016913	0.029280
C	2.103122	1.348045	0.016082
H	-2.180534	2.564661	0.028382
N	-1.508323	1.812189	0.020987
O	1.312219	2.297449	0.034850
C	3.953234	-0.834758	-0.027746
C	4.940893	-1.965115	-0.050568
C	-1.965598	0.552976	0.006986
N	1.707722	0.034325	-0.004575
N	-1.092526	-0.486206	-0.002294

C	2.607808	-1.007414	-0.025515
C	-3.346291	0.242312	0.001083
N	-4.471500	1.045272	0.007451
H	0.679698	-0.155419	-0.003412
C	-1.570553	-1.747499	-0.016074
H	4.425368	-2.931173	-0.065441
H	-0.815396	-2.530496	-0.022522
C	-3.685488	-1.112717	-0.013589
H	2.159285	-1.995590	-0.040487
C	-5.470728	0.194385	-0.003223
N	-2.837690	-2.155727	-0.022648
H	-6.519065	0.461211	-0.002323
N	-5.060763	-1.125422	-0.016213
H	-5.645440	-1.948769	-0.025983
H	5.589887	-1.893393	-0.931139

AT-ST1, C_1, **E=-921.568115237**

N	1.267556	1.194647	-1.025065
H	1.616885	0.872760	-1.920493
C	2.114090	1.015349	0.051966
O	3.255929	0.579532	-0.041843
N	1.537741	1.369001	1.259297
H	2.110124	1.217767	2.077376
C	0.232782	1.799722	1.387199
H	-0.083662	2.017139	2.400920
C	-0.598367	1.934220	0.327136
C	-0.085158	1.581194	-0.997454
O	-0.737437	1.602431	-2.036582
C	-2.025566	2.379239	0.448371
H	-2.226437	2.760740	1.454725
H	-2.702694	1.538040	0.261752
H	-2.247016	3.161503	-0.285404

H	-3.387443	-0.408761	-1.342328
N	-2.507348	-0.881735	-1.494431
H	-2.012228	-0.645568	-2.344974
C	-1.746102	-1.099231	-0.393984
N	-2.289869	-0.942098	0.829328
C	-1.508742	-1.119683	1.907494
H	-1.998300	-0.970301	2.867066
N	-0.209788	-1.443836	1.956347
C	0.292038	-1.632322	0.728354
N	1.572198	-1.980404	0.364294
H	2.368122	-2.067005	0.979492
C	1.597656	-2.016733	-1.013506
H	2.507502	-2.245413	-1.551053
N	0.438287	-1.738879	-1.563027
C	-0.393883	-1.494925	-0.485172

B. ωB97X-D/6-31+G(d,p) geometries of neutral dimers

TT-HB1, C_{2h}, E=-908.075571779

H	3.123694	2.429811	0.000000
H	-2.740471	2.322106	0.000000
H	-5.178272	2.618159	0.000000
H	-6.026172	1.326457	0.878301
O	5.340843	1.344823	0.000000
N	3.069637	1.418965	0.000000
O	0.796479	1.585913	0.000000
C	-5.413759	1.550972	0.000000
C	-2.916661	1.252033	0.000000
H	-0.843456	0.925699	0.000000
C	4.290474	0.727246	0.000000
C	1.808498	0.879295	0.000000
H	-6.026172	1.326457	-0.878301

C	-4.160999	0.730082	0.000000
N	-1.775295	0.483412	0.000000
N	1.775295	-0.483412	0.000000
C	4.160999	-0.730082	0.000000
H	6.026172	-1.326457	-0.878301
C	-1.808498	-0.879295	0.000000
C	-4.290474	-0.727246	0.000000
H	0.843456	-0.925699	0.000000
C	2.916661	-1.252033	0.000000
C	5.413759	-1.550972	0.000000
O	-0.796479	-1.585913	0.000000
N	-3.069637	-1.418965	0.000000
O	-5.340843	-1.344823	0.000000
H	6.026172	-1.326457	0.878301
H	5.178272	-2.618159	0.000000
H	2.740471	-2.322106	0.000000
H	-3.123694	-2.429811	0.000000

TT-HB2, C_s, E=-908.069633769

N	2.878410	1.364155	0.000000
H	2.971923	2.372119	0.000000
C	1.593837	0.874767	0.000000
O	0.611281	1.614419	0.000000
N	1.508857	-0.488466	0.000000
H	0.555500	-0.879287	0.000000
C	2.616872	-1.302228	0.000000
H	2.397172	-2.364363	0.000000
C	3.880712	-0.828933	0.000000
C	4.067760	0.622733	0.000000
O	5.144569	1.194872	0.000000
C	5.103069	-1.695524	0.000000
H	4.831705	-2.754283	0.000000

H	5.721724	-1.491015	0.878629
H	5.721724	-1.491015	-0.878629
O	-3.008857	2.755666	0.000000
C	-3.129091	1.548305	0.000000
N	-4.367198	0.923897	0.000000
H	-5.160373	1.547110	0.000000
C	-4.534091	-0.437966	0.000000
H	-5.563175	-0.780614	0.000000
C	-3.490219	-1.292516	0.000000
N	-2.066931	0.661971	0.000000
H	-1.122217	1.081477	0.000000
C	-2.148262	-0.716886	0.000000
O	-1.126411	-1.410311	0.000000
C	-3.628444	-2.784619	0.000000
H	-4.681168	-3.078473	0.000000
H	-3.144551	-3.219450	0.879254
H	-3.144551	-3.219450	-0.879254

TT-HB3, C_s, E=-908.068551941

N	1.984407	0.170818	0.000000
H	1.098231	0.701109	0.000000
C	1.875851	-1.189503	0.000000
O	0.804097	-1.799110	0.000000
N	3.071508	-1.863734	0.000000
H	3.003062	-2.869711	0.000000
C	4.298934	-1.230140	0.000000
H	5.159147	-1.890152	0.000000
C	4.411443	0.110045	0.000000
C	3.176918	0.909922	0.000000
O	3.151061	2.125691	0.000000
C	5.716789	0.843817	0.000000
H	6.559943	0.148479	0.000000

H	5.792227	1.491409	0.878088
H	5.792227	1.491409	-0.878088
O	-0.586681	1.401808	0.000000
C	-1.648066	0.781932	0.000000
N	-1.723175	-0.582498	0.000000
H	-0.824406	-1.082605	0.000000
C	-2.918605	-1.261545	0.000000
H	-2.824529	-2.342067	0.000000
C	-4.118605	-0.644487	0.000000
N	-2.867556	1.416702	0.000000
H	-2.842917	2.428770	0.000000
C	-4.135350	0.819285	0.000000
O	-5.138119	1.512817	0.000000
C	-5.432740	-1.363955	0.000000
H	-5.285401	-2.446965	0.000000
H	-6.024060	-1.089894	-0.878639
H	-6.024060	-1.089894	0.878639

TT-ST1, C_2, E=-908.063157016

H	-1.654653	-2.325812	-2.803258
H	1.701709	-2.088830	-1.651434
C	0.936165	-1.899881	-0.907505
H	2.357581	-1.986170	0.604055
C	-0.345575	-1.649157	-1.242267
N	1.372238	-1.924722	0.395351
C	-1.290856	-1.351844	-0.164640
C	0.560199	-1.649926	1.476267
N	-0.758661	-1.425449	1.124628
O	0.970518	-1.600167	2.619975
O	-2.459698	-1.034329	-0.330158
H	-1.376235	-1.182561	1.891051
C	-0.848669	-1.602597	-2.650666

H	-0.048120	-1.819390	-3.362530
H	-1.257560	-0.612687	-2.879041
H	1.654653	2.325812	-2.803258
H	-1.701709	2.088830	-1.651434
C	-0.936165	1.899881	-0.907505
H	-2.357581	1.986170	0.604055
C	0.345575	1.649157	-1.242267
N	-1.372238	1.924722	0.395351
C	1.290856	1.351844	-0.164640
C	-0.560199	1.649926	1.476267
N	0.758661	1.425449	1.124628
O	-0.970518	1.600167	2.619975
O	2.459698	1.034329	-0.330158
H	1.376235	1.182561	1.891051
C	0.848669	1.602597	-2.650666
H	0.048120	1.819390	-3.362530
H	1.257560	0.612687	-2.879041

TT-ST3, C_1, E=-908.061137096

N	0.576233	-1.664965	-0.480344
H	-0.053338	-2.209599	-1.059486
C	0.555176	-1.941261	0.868801
O	-0.190639	-2.761255	1.379388
N	1.455756	-1.189717	1.592680
H	1.472525	-1.372421	2.583931
C	2.216123	-0.177039	1.042847
H	2.833129	0.372975	1.744407
C	2.186835	0.126853	-0.269110
C	1.324491	-0.680087	-1.138708
O	1.214905	-0.535980	-2.343113
C	2.935633	1.265131	-0.889481

H	3.466007	0.931799	-1.784984
H	3.653422	1.691560	-0.184132
H	2.229829	2.046982	-1.188616
O	-0.159976	2.686295	-0.602744
C	-0.823963	1.717502	-0.268826
N	-1.420957	0.902537	-1.233548
H	-1.185272	1.100369	-2.199114
C	-2.124434	-0.266769	-1.022407
O	-2.511083	-0.995170	-1.917037
N	-2.341448	-0.540888	0.313833
H	-2.771790	-1.434063	0.503578
C	-1.785023	0.191132	1.335324
H	-1.972702	-0.196403	2.330455
C	-1.049002	1.300010	1.117812
C	-0.420528	2.107971	2.210397
H	-0.637797	1.673525	3.189924
H	-0.788785	3.137519	2.196820
H	0.665343	2.156836	2.079104

AA-HB1, C_{2h}, **E=-934.424896814**

H	6.292227	0.890958	0.000000
H	2.339134	2.998012	0.000000
N	3.918537	1.682204	0.000000
C	2.608740	1.945393	0.000000
N	5.635824	0.128558	0.000000
H	5.959851	-0.823957	0.000000
C	4.316519	0.399099	0.000000
H	-1.836308	3.401824	0.000000
N	1.592843	1.083553	0.000000
C	-2.170176	2.373703	0.000000
H	-0.233235	1.389052	0.000000

C	3.340105	-0.614417	0.000000
C	2.013229	-0.195274	0.000000
N	-1.269104	1.340605	0.000000
N	-3.423464	1.990687	0.000000
N	3.423464	-1.990687	0.000000
C	-2.013229	0.195274	0.000000
N	1.269104	-1.340605	0.000000
C	-3.340105	0.614417	0.000000
C	2.170176	-2.373703	0.000000
H	-5.959851	0.823957	0.000000
H	0.233235	-1.389052	0.000000
N	-1.592843	-1.083553	0.000000
C	-4.316519	-0.399099	0.000000
H	1.836308	-3.401824	0.000000
N	-5.635824	-0.128558	0.000000
C	-2.608740	-1.945393	0.000000
H	-6.292227	-0.890958	0.000000
N	-3.918537	-1.682204	0.000000
H	-2.339134	-2.998012	0.000000

AA-ST1, C_1, E=-934.408777099

H	-2.916999	-2.731286	-0.543370
C	-2.480246	-1.824758	-0.132243
H	0.216295	-2.180367	-2.187656
N	-1.503928	-2.017795	0.764904
N	-2.974537	-0.677846	-0.591885
H	-0.821742	-0.030911	-3.082264
N	0.508073	-1.252572	-1.923979
C	-0.034938	-0.062209	-2.341655
C	-0.920485	-0.944972	1.320499
H	0.484945	-2.048177	2.249084
C	-2.376897	0.372176	-0.015812

N	2.228405	-1.772387	-0.270667
C	1.451341	-0.943766	-0.978029
N	0.064407	-1.131811	2.228166
C	-1.368497	0.335402	0.942780
H	-3.248486	2.101850	-0.894997
N	-2.595445	1.706853	-0.237840
N	0.487136	0.983234	-1.756315
C	1.420923	0.445625	-0.890738
H	0.653071	-0.345872	2.459347
C	2.992937	-1.105599	0.587696
H	3.655194	-1.708763	1.202643
N	-0.965355	1.609591	1.298087
C	-1.718849	2.389184	0.568661
N	3.042735	0.216187	0.814564
C	2.261454	1.020605	0.079867
H	-1.690578	3.469705	0.578811
H	1.541606	2.907246	-0.040244
N	2.321448	2.358324	0.285654
H	2.775300	2.658718	1.134250

AT-HB1, C_1, E=-921.249871309

H	5.990803	0.257317	0.022081
H	5.818089	1.996776	0.019878
N	5.408734	1.077898	0.018515
C	4.068240	0.951483	0.010265
N	3.921234	-1.597346	0.010377
N	3.309286	2.059605	0.004809
C	3.436302	-0.306013	0.006972
C	2.837151	-2.333854	0.003994
H	2.826114	-3.414466	0.004252
C	1.980368	1.923672	-0.003002

C	2.046147	-0.297451	-0.001553
H	1.418902	2.854082	-0.006910
N	1.672730	-1.609751	-0.003636
N	1.265444	0.799213	-0.006820
H	0.700287	-1.942154	-0.007443
H	-0.542536	0.457785	-0.008091
O	-1.098938	-2.021548	-0.008926
N	-1.553949	0.224876	-0.003087
C	-1.909541	-1.093193	-0.001881
H	-2.061023	2.237800	0.005091
C	-2.483575	1.238850	0.006327
H	-5.469074	2.039790	0.929522
N	-3.265118	-1.316144	0.007929
H	-3.561108	-2.284059	0.008495
C	-3.816446	1.028743	0.017057
C	-4.286487	-0.355709	0.017988
H	-4.386136	3.104177	0.006639
C	-4.848363	2.114461	0.031437
O	-5.453516	-0.708587	0.026497
H	-5.521817	2.015732	-0.824744

AT-HB2, C_1, E=-921.245230697

H	5.596527	-2.096650	0.714471
H	3.837722	2.289344	0.026343
O	5.628520	0.597748	-0.053572
N	3.483834	1.341208	0.026773
C	4.441143	0.320560	-0.017935
H	-0.474959	2.024875	0.045640
C	2.116653	1.203029	0.065907
H	-2.114061	2.657717	-0.040449
N	-1.485589	1.872475	0.005393
O	1.363330	2.174479	0.097274

C	3.886107	-1.032867	-0.016898
C	4.846983	-2.180740	-0.077021
C	-2.000728	0.640100	0.020912
N	1.678899	-0.091800	0.067295
N	-1.185329	-0.435293	0.085738
C	2.542566	-1.160462	0.025227
C	-3.391341	0.398192	-0.025435
N	-4.471134	1.255994	-0.088479
H	0.649890	-0.235262	0.086886
C	-1.728456	-1.666476	0.104910
H	4.328489	-3.137512	0.025133
H	-1.012881	-2.483164	0.162822
C	-3.798588	-0.928865	0.000576
H	2.064411	-2.134167	0.027521
C	-5.505937	0.458463	-0.100192
N	-3.006261	-2.010519	0.067697
H	-6.535738	0.784039	-0.138755
N	-5.166911	-0.873773	-0.049083
H	-5.790891	-1.664766	-0.045310
H	5.386351	-2.178975	-1.029256

AT-ST1, C_1, E=-921.238057177

N	-1.214339	1.260338	-1.023434
H	-1.551031	0.934653	-1.921020
C	-2.084000	1.115243	0.034383
O	-3.223952	0.693180	-0.077565
N	-1.538013	1.491061	1.242124
H	-2.133390	1.370755	2.046578
C	-0.231527	1.901523	1.390783
H	0.066355	2.135902	2.406656
C	0.624041	2.001622	0.354690
C	0.132020	1.637210	-0.975597

O	0.800308	1.645098	-1.997204
C	2.053856	2.424780	0.488921
H	2.254592	2.809056	1.492282
H	2.294166	3.200282	-0.242895
H	2.723628	1.577967	0.308399
N	2.281882	-1.072072	0.796537
C	1.510831	-1.233238	1.881076
H	2.014858	-1.102651	2.835016
N	0.212992	-1.524914	1.944781
C	-0.308957	-1.685764	0.723133
C	1.725717	-1.219341	-0.415690
N	2.484869	-1.041144	-1.519210
H	3.379062	-0.595028	-1.387932
H	2.002727	-0.849072	-2.384805
N	-1.601068	-1.987826	0.375253
H	-2.389298	-2.060366	0.998632
C	-1.643393	-2.019601	-0.996894
H	-2.566182	-2.213291	-1.525099
N	-0.488078	-1.779949	-1.558744
C	0.363001	-1.567721	-0.490774

C. ωB97X-D geometries of dimers cations

TT-HB1, C_{2h}, E=-907.752611398

H	3.093753	2.421110	0.000000
H	-2.752550	2.370958	0.000000
H	-5.214864	2.617966	0.000000
H	-6.029133	1.293497	0.873923
O	5.324711	1.331217	0.000000
N	3.049840	1.407144	0.000000
O	0.770728	1.501876	0.000000
C	-5.418064	1.546277	0.000000

C	-2.910135	1.297938	0.000000
H	-0.847525	0.967735	0.000000
C	4.279254	0.724592	0.000000
C	1.810517	0.846430	0.000000
H	-6.029133	1.293497	-0.873923
C	-4.167494	0.747727	0.000000
N	-1.790687	0.537614	0.000000
N	1.790687	-0.537614	0.000000
C	4.167494	-0.747727	0.000000
H	6.029133	-1.293497	-0.873923
C	-1.810517	-0.846430	0.000000
C	-4.279254	-0.724592	0.000000
H	0.847525	-0.967735	0.000000
C	2.910135	-1.297938	0.000000
C	5.418064	-1.546277	0.000000
O	-0.770728	-1.501876	0.000000
N	-3.049840	-1.407144	0.000000
O	-5.324711	-1.331217	0.000000
H	6.029133	-1.293497	0.873923
H	5.214864	-2.617966	0.000000
H	2.752550	-2.370958	0.000000
H	-3.093753	-2.421110	0.000000

TT-HB1 (HT), C_s, E=-907.768761357

H	2.959622	2.429451	0.000000
H	-2.613327	2.285275	0.000000
H	-5.044305	2.629404	0.000000
H	-5.923094	1.339985	0.872123
O	5.214827	1.417794	0.000000
N	2.941197	1.414360	0.000000
O	0.695978	1.545897	0.000000
C	-5.298614	1.569132	0.000000

C	-2.774969	1.209228	0.000000
H	-0.208921	1.060119	0.000000
C	4.207737	0.755634	0.000000
C	1.753348	0.803516	0.000000
H	-5.923094	1.339985	-0.872123
C	-4.098165	0.708461	0.000000
N	-1.698909	0.455872	0.000000
N	1.723427	-0.525427	0.000000
C	4.119479	-0.710099	0.000000
H	5.999087	-1.221454	-0.878931
C	-1.820167	-0.943954	0.000000
C	-4.270808	-0.757548	0.000000
H	0.806000	-1.000721	0.000000
C	2.898985	-1.276182	0.000000
C	5.402223	-1.479734	0.000000
O	-0.816567	-1.643932	0.000000
N	-3.076117	-1.481033	0.000000
O	-5.348675	-1.308595	0.000000
H	5.999087	-1.221454	0.878931
H	5.216806	-2.555093	0.000000
H	2.742751	-2.347862	0.000000
H	-3.149428	-2.493716	0.000000

TT-HB2 (HT), C_s, E=-907.772568263

N	2.881486	1.414827	0.000000
H	2.991071	2.424249	0.000000
C	1.604187	0.925200	0.000000
O	0.628645	1.660198	0.000000
N	1.429023	-0.469268	0.000000
H	-0.115728	-0.985325	0.000000
C	2.475419	-1.262489	0.000000

H	2.273497	-2.331737	0.000000
C	3.816157	-0.812097	0.000000
C	4.045859	0.646726	0.000000
O	5.145921	1.153294	0.000000
C	4.984200	-1.717153	0.000000
H	4.690127	-2.767190	0.000000
H	5.616411	-1.511907	0.872237
H	5.616411	-1.511907	-0.872237
O	-2.917228	2.745237	0.000000
C	-3.053105	1.550885	0.000000
N	-4.280935	0.903338	0.000000
H	-5.088100	1.514627	0.000000
C	-4.429390	-0.446015	0.000000
H	-5.452049	-0.806879	0.000000
C	-3.367648	-1.300783	0.000000
N	-1.972996	0.655236	0.000000
H	-1.035632	1.099857	0.000000
C	-2.083453	-0.685518	0.000000
O	-1.032704	-1.437619	0.000000
C	-3.495769	-2.796644	0.000000
H	-4.547315	-3.088869	0.000000
H	-3.019664	-3.231013	0.882770
H	-3.019664	-3.231013	-0.882770

TT-HB3, C_s, E=-907.765300784

N	1.982995	0.336887	0.000000
H	1.177321	0.961613	0.000000
C	1.749734	-0.994481	0.000000
O	0.601682	-1.502683	0.000000
N	2.847158	-1.784077	0.000000
H	2.683438	-2.780596	0.000000

C	4.141671	-1.278115	0.000000
H	4.923199	-2.028234	0.000000
C	4.396267	0.042591	0.000000
C	3.255241	0.966111	0.000000
O	3.319009	2.173879	0.000000
C	5.771255	0.633875	0.000000
H	6.535278	-0.145754	0.000000
H	5.912988	1.268562	0.878761
H	5.912988	1.268562	-0.878761
O	-0.739853	1.646942	0.000000
C	-1.752780	0.989377	0.000000
N	-1.673594	-0.429438	0.000000
H	-0.629058	-0.850833	0.000000
C	-2.727985	-1.213696	0.000000
H	-2.538408	-2.283970	0.000000
C	-4.042799	-0.701945	0.000000
N	-3.020587	1.504234	0.000000
H	-3.100840	2.517236	0.000000
C	-4.209952	0.773757	0.000000
O	-5.291981	1.311065	0.000000
C	-5.246023	-1.553494	0.000000
H	-5.003603	-2.616171	0.000000
H	-5.869824	-1.314037	-0.870790
H	-5.869824	-1.314037	0.870790

TT-HB3 (HT), C_s, E=-907.766423373

N	1.923008	0.158207	0.000000
H	1.062263	0.731465	0.000000
C	1.813027	-1.168043	0.000000
O	0.692179	-1.805816	0.000000
N	2.931371	-1.899715	0.000000

H	2.826844	-2.905556	0.000000
C	4.196603	-1.314348	0.000000
H	5.021553	-2.015753	0.000000
C	4.360932	0.019910	0.000000
C	3.163236	0.871850	0.000000
O	3.147021	2.076484	0.000000
C	5.692202	0.702082	0.000000
H	6.508078	-0.022564	0.000000
H	5.787260	1.345324	0.878834
H	5.787260	1.345324	-0.878834
O	-0.573886	1.449374	0.000000
C	-1.622682	0.826562	0.000000
N	-1.601951	-0.580872	0.000000
H	-0.184260	-1.248184	0.000000
C	-2.727220	-1.258004	0.000000
H	-2.641153	-2.342684	0.000000
C	-4.010819	-0.664901	0.000000
N	-2.841308	1.448769	0.000000
H	-2.841574	2.464258	0.000000
C	-4.081558	0.810786	0.000000
O	-5.120926	1.431878	0.000000
C	-5.268284	-1.440222	0.000000
H	-5.087986	-2.515622	0.000000
H	-5.875507	-1.168793	-0.872141
H	-5.875507	-1.168793	0.872141

TT-ST1, C_1, E=-907.752083055

N	0.118342	-1.840558	0.751443
H	-0.507200	-2.320123	1.391835
C	0.055875	-2.255484	-0.564076
O	-0.709894	-3.077966	-0.992752

N	0.973832	-1.588836	-1.401197
H	0.923825	-1.851278	-2.380016
C	1.845978	-0.661886	-0.980644
H	2.510821	-0.253154	-1.734744
C	1.883708	-0.233458	0.333178
C	0.950869	-0.860732	1.288760
O	0.862708	-0.535064	2.456659
C	2.951585	0.664803	0.857947
H	3.470431	1.187543	0.052379
H	3.685590	0.071043	1.414863
H	2.547867	1.387506	1.570669
O	-3.146856	-0.330596	1.054680
C	-2.244398	0.318013	0.596248
N	-1.445380	1.152705	1.408337
H	-1.685438	1.140859	2.394374
C	-0.422521	1.888242	0.957437
H	0.094347	2.495112	1.693632
C	-0.018885	1.858366	-0.367195
N	-1.857084	0.319226	-0.727611
H	-2.412779	-0.263101	-1.347002
C	-0.780417	0.997858	-1.294160
O	-0.486679	0.840782	-2.463115
C	0.996719	2.801127	-0.915375
H	1.721965	3.098853	-0.155391
H	0.504045	3.708489	-1.285188
H	1.508729	2.357194	-1.770854

TT-ST1, C_2, E=-907.751460725

H	2.794949	0.447566	-2.816802
H	0.436551	2.439750	-1.825625
C	0.766152	1.802468	-1.011249
H	0.027757	3.127466	0.372974

C	1.369893	0.579481	-1.240256
N	0.542360	2.265346	0.225656
C	1.786303	-0.209846	-0.065954
C	0.905858	1.585571	1.407305
N	1.557633	0.393093	1.168810
O	0.638563	2.022484	2.495541
O	2.256787	-1.329226	-0.137578
H	1.843002	-0.125325	1.994749
C	1.770586	0.120628	-2.600764
H	1.118782	0.535593	-3.372958
H	1.772075	-0.969310	-2.653394
H	-2.794949	-0.447566	-2.816802
H	-0.436551	-2.439750	-1.825625
C	-0.766152	-1.802468	-1.011249
H	-0.027757	-3.127466	0.372974
C	-1.369893	-0.579481	-1.240256
N	-0.542360	-2.265346	0.225656
C	-1.786303	0.209846	-0.065954
C	-0.905858	-1.585571	1.407305
N	-1.557633	-0.393093	1.168810
O	-0.638563	-2.022484	2.495541
O	-2.256787	1.329226	-0.137578
H	-1.843002	0.125325	1.994749
C	-1.770586	-0.120628	-2.600764
H	-1.118782	-0.535593	-3.372958
H	-1.772075	0.969310	-2.653394

TT-ST3, C_1, E=-907.752511006

N	0.993683	-1.482450	0.936212
H	0.576012	-2.408323	0.961896
C	0.436375	-0.550785	1.771461
O	-0.493445	-0.727113	2.512224

N	1.067077	0.727743	1.700670
H	0.685244	1.411208	2.347661
C	2.036782	1.048573	0.852601
H	2.416612	2.064113	0.885020
C	2.538335	0.112458	-0.061901
C	1.980610	-1.264556	-0.028723
O	2.335120	-2.139321	-0.780697
C	3.585648	0.432745	-1.045176
H	4.364991	-0.336470	-1.034453
H	4.018913	1.420115	-0.885830
H	3.139021	0.399421	-2.047787
O	0.530280	0.892573	-1.445445
C	-0.614701	0.664761	-1.029665
N	-1.160100	-0.596357	-1.195216
H	-0.633556	-1.259008	-1.754228
C	-2.361773	-1.067023	-0.680221
O	-2.749541	-2.201623	-0.813243
N	-3.054886	-0.090117	0.024723
H	-3.933566	-0.391797	0.425499
C	-2.618280	1.188693	0.182310
H	-3.279433	1.838922	0.744759
C	-1.428981	1.627032	-0.314587
C	-0.955342	3.046830	-0.222859
H	-1.612510	3.647698	0.408182
H	-0.921048	3.500580	-1.217228
H	0.060937	3.104325	0.178643

AA-HB1, C_{2h}, E= -934.121593981

H	6.286758	0.903525	0.000000
H	2.339021	2.987947	0.000000
N	3.917128	1.682725	0.000000

C	2.621043	1.939690	0.000000
N	5.629609	0.135705	0.000000
H	5.968377	-0.815972	0.000000
C	4.327881	0.396879	0.000000
H	-1.847948	3.413041	0.000000
N	1.590517	1.058617	0.000000
C	-2.164662	2.379538	0.000000
H	-0.229863	1.410390	0.000000
C	3.344531	-0.632003	0.000000
C	2.001305	-0.203464	0.000000
N	-1.265635	1.358113	0.000000
N	-3.431609	1.981608	0.000000
N	3.431609	-1.981608	0.000000
C	-2.001305	0.203464	0.000000
N	1.265635	-1.358113	0.000000
C	-3.344531	0.632003	0.000000
C	2.164662	-2.379538	0.000000
H	-5.968377	0.815972	0.000000
H	0.229863	-1.410390	0.000000
N	-1.590517	-1.058617	0.000000
C	-4.327881	-0.396879	0.000000
H	1.847948	-3.413041	0.000000
N	-5.629609	-0.135705	0.000000
C	-2.621043	-1.939690	0.000000
H	-6.286758	-0.903525	0.000000
N	-3.917128	-1.682725	0.000000
H	-2.339021	-2.987947	0.000000

AA-HB1, C_2, E=-934.121562402

H	6.290986	0.874249	0.000102
H	2.352451	2.976785	0.000090
N	3.924597	1.664578	0.000079

C	2.629641	1.927232	0.000049
N	5.630094	0.109639	0.000095
H	5.964390	-0.843628	0.000084
C	4.329609	0.376981	0.000092
H	-1.833176	3.422066	0.000049
N	1.595237	1.050708	0.000056
C	-2.154294	2.389929	0.000052
H	-0.223774	1.412330	0.000093
C	3.341772	-0.647557	0.000066
C	2.000459	-0.213219	0.000055
N	-1.259719	1.364624	0.000072
N	-3.422977	1.997536	0.000044
N	3.422977	-1.997536	0.000044
C	-2.000459	0.213219	0.000055
N	1.259719	-1.364624	0.000072
C	-3.341772	0.647557	0.000066
C	2.154294	-2.389929	0.000052
H	-5.964390	0.843628	0.000084
H	0.223774	-1.412330	0.000093
N	-1.595237	-1.050708	0.000056
C	-4.329609	-0.376981	0.000092
H	1.833176	-3.422066	0.000049
N	-5.630094	-0.109639	0.000095
C	-2.629641	-1.927232	0.000049
H	-6.290986	-0.874249	0.000102
N	-3.924597	-1.664578	0.000079
H	-2.352451	-2.976785	0.000090

AA-HB1 (HT), C_s, E=-934.147880064

H	5.951495	-0.781139	0.000000
H	6.245414	0.940866	0.000000
N	5.600369	0.164946	0.000000

N	3.432391	-1.997299	0.000000
H	1.879395	-3.446834	0.000000
C	4.295107	0.401180	0.000000
C	2.194459	-2.413314	0.000000
C	3.326312	-0.626591	0.000000
N	3.875959	1.695961	0.000000
N	1.267098	-1.389651	0.000000
C	1.993648	-0.249990	0.000000
H	0.234958	-1.444336	0.000000
C	2.596527	1.965169	0.000000
N	1.603649	1.048863	0.000000
H	2.280293	3.002618	0.000000
H	-2.364991	-2.968352	0.000000
N	-1.607546	-1.036975	0.000000
C	-2.649572	-1.920570	0.000000
H	0.588934	1.306635	0.000000
C	-1.986595	0.224130	0.000000
N	-1.204417	1.358629	0.000000
N	-3.944140	-1.670396	0.000000
C	-3.361274	0.650442	0.000000
C	-2.099764	2.334425	0.000000
C	-4.353078	-0.382794	0.000000
H	-1.816742	3.379480	0.000000
N	-3.438184	1.966415	0.000000
N	-5.648106	-0.116516	0.000000
H	-6.310809	-0.880913	0.000000
H	-5.981413	0.838117	0.000000

AA-ST1, C_1, E=-934.127742858

H	-2.499751	-2.058127	-1.169487
C	-2.102286	-1.304518	-0.496126
H	0.989228	-2.992083	-2.031044

N	-1.253127	-1.738172	0.427022
N	-2.544948	-0.044563	-0.707022
H	-0.378651	-1.434902	-3.512054
N	0.918535	-1.992674	-1.901765
C	0.184061	-1.117798	-2.644663
C	-0.756728	-0.850554	1.315021
H	0.297304	-2.262275	2.319334
C	-2.030921	0.812329	0.149505
N	2.292362	-1.667471	0.079481
C	1.496037	-1.267775	-0.889674
N	0.078490	-1.277214	2.259845
C	-1.133407	0.513992	1.197982
H	-2.834157	2.729101	-0.327092
N	-2.225409	2.168461	0.252090
N	0.249799	0.131824	-2.211857
C	1.058318	0.057308	-1.124385
H	0.433176	-0.636914	2.956672
C	2.682571	-0.640757	0.867278
H	3.352172	-0.902824	1.681072
N	-0.807784	1.621699	1.910624
C	-1.475426	2.591523	1.312361
N	2.381861	0.649742	0.759117
C	1.578302	1.043574	-0.242548
H	-1.465359	3.624401	1.632023
H	0.830154	2.676753	-1.206489
N	1.293811	2.343312	-0.374177
H	1.781997	2.996986	0.221390

AT-HB1, C_1, E=-920.953289070

H	6.128814	-0.039118	-0.002938
H	6.133910	1.714059	-0.005838

N	5.623539	0.838429	-0.003711
C	4.305740	0.862016	-0.001991
N	3.834897	-1.627220	0.002410
N	3.667166	2.056044	-0.003178
C	3.519195	-0.337452	0.001115
C	2.623857	-2.246128	0.004130
H	2.515002	-3.322489	0.005458
C	2.352815	2.071391	-0.001737
C	2.099272	-0.145119	0.001930
H	1.887175	3.051415	-0.002387
N	1.575556	-1.416002	0.003899
N	1.483021	1.006269	0.000645
H	0.513624	-1.629678	0.004214
H	-0.692102	0.700528	-0.000983
O	-0.960737	-1.808546	0.005329
N	-1.656170	0.378308	0.001095
C	-1.875418	-0.962583	0.004027
H	-2.363091	2.340680	-0.001634
C	-2.689250	1.307428	0.000102
H	-5.755966	1.772550	0.878371
N	-3.180358	-1.336556	0.005464
H	-3.370516	-2.332126	0.007604
C	-3.985493	0.950070	0.001532
C	-4.307303	-0.482640	0.004185
H	-4.754670	2.952749	0.000063
C	-5.121732	1.924770	0.000659
O	-5.421240	-0.956617	0.005360
H	-5.755666	1.771444	-0.877091

AT-HB1 (HT: $AH^+(T–H)^\bullet$), C_s, E=-920.967582809

H	5.988546	0.428643	0.000000
H	5.708269	2.152984	0.000000

N	5.349219	1.209813	0.000000
C	4.040368	1.001413	0.000000
N	4.037830	-1.545255	0.000000
N	3.210888	2.080716	0.000000
C	3.473459	-0.292255	0.000000
C	3.017296	-2.359180	0.000000
H	3.072735	-3.438121	0.000000
C	1.917403	1.902643	0.000000
C	2.091676	-0.389821	0.000000
H	1.273787	2.776019	0.000000
N	1.798885	-1.708103	0.000000
N	1.288882	0.704888	0.000000
H	0.856172	-2.095849	0.000000
H	0.252112	0.635000	0.000000
O	-1.028553	-1.822292	0.000000
N	-1.598258	0.385166	0.000000
C	-1.917008	-0.983865	0.000000
H	-2.262629	2.316712	0.000000
C	-2.566690	1.271584	0.000000
H	-5.666726	1.841424	0.871275
N	-3.240864	-1.343566	0.000000
H	-3.453442	-2.335745	0.000000
C	-3.945967	0.961273	0.000000
C	-4.322383	-0.464130	0.000000
H	-4.615386	2.995954	0.000000
C	-5.015688	1.981890	0.000000
O	-5.468289	-0.859836	0.000000
H	-5.666726	1.841424	-0.871275

AT-HB2, C_1, E=-920.950866853

H	5.820832	-1.859673	0.857083
H	3.603902	2.328683	-0.029371

O	5.593506	0.868684	-0.028678
N	3.371015	1.342274	-0.023379
C	4.460351	0.441643	-0.022927
H	-0.329320	1.725426	-0.021661
C	2.051664	1.020782	-0.016190
H	-1.955158	2.533095	-0.037999
N	-1.409473	1.676754	-0.024231
O	1.165668	1.895180	-0.017107
C	4.079015	-0.976295	-0.015933
C	5.177897	-1.992956	-0.017398
C	-2.043980	0.533660	-0.006660
N	1.776600	-0.309569	-0.008143
N	-1.328936	-0.636312	0.013296
C	2.768692	-1.279759	-0.008449
C	-3.475208	0.443162	-0.006071
N	-4.436572	1.376363	-0.019362
H	0.792412	-0.568950	0.002497
C	-1.979293	-1.776855	0.030865
H	4.777096	-3.008312	-0.013513
H	-1.382882	-2.683659	0.048042
C	-4.014463	-0.875151	0.012426
H	2.404811	-2.300421	-0.003498
C	-5.569717	0.670596	-0.009380
N	-3.335790	-1.986741	0.031553
H	-6.558726	1.108135	-0.014600
N	-5.377895	-0.671803	0.009073
H	-6.091085	-1.389629	0.019466
H	5.813717	-1.864145	-0.897749

AT-HB2 (HT), C_1, E=–920.969256827

H	5.603575	-2.043166	0.944969
H	3.782062	2.315498	-0.030253

O	5.680893	0.697188	-0.018233
N	3.495608	1.341964	-0.027657
C	4.509033	0.386233	-0.020191
H	-0.497877	2.080638	-0.020792
C	2.149588	1.080929	-0.028952
H	-2.143707	2.713805	-0.006652
N	-1.509087	1.928195	-0.012283
O	1.325352	1.983017	-0.031682
C	4.028410	-1.007437	-0.014415
C	5.026321	-2.098155	0.012882
C	-2.020375	0.711433	-0.009894
N	1.727376	-0.259659	-0.027561
N	-1.217098	-0.392993	-0.018247
C	2.629619	-1.213886	-0.020663
C	-3.396907	0.416447	0.000803
N	-4.483094	1.253539	0.010600
H	-0.186310	-0.288048	-0.024729
C	-1.707560	-1.673902	-0.016599
H	4.565440	-3.083626	-0.061983
H	-0.951903	-2.451447	-0.024338
C	-3.780133	-0.919888	0.001471
H	2.254344	-2.235483	-0.019580
C	-5.505821	0.437546	0.017010
N	-2.963640	-1.997870	-0.007317
H	-6.541434	0.745692	0.024460
N	-5.139082	-0.888711	0.012052
H	-5.752532	-1.691286	0.015346
H	5.757437	-1.962137	-0.791239

AT-HB2 (HT), C_s, E=-920.969249856

H	5.669254	-1.963821	0.871108
H	3.746051	2.340404	0.000000

O	5.651601	0.730030	0.000000
N	3.463679	1.365668	0.000000
C	4.481069	0.414172	0.000000
H	-0.534671	2.085113	0.000000
C	2.118830	1.098594	0.000000
H	-2.183658	2.709939	0.000000
N	-1.545064	1.927523	0.000000
O	1.290530	1.996965	0.000000
C	4.006603	-0.981678	0.000000
C	5.011067	-2.066459	0.000000
C	-2.050102	0.708136	0.000000
N	1.702571	-0.243886	0.000000
N	-1.240604	-0.391835	0.000000
C	2.608875	-1.194411	0.000000
C	-3.424987	0.405442	0.000000
N	-4.516186	1.236399	0.000000
H	-0.210366	-0.281394	0.000000
C	-1.723937	-1.675368	0.000000
H	4.554892	-3.056762	0.000000
H	-0.964218	-2.448994	0.000000
C	-3.800726	-0.932987	0.000000
H	2.237651	-2.217455	0.000000
C	-5.534301	0.414489	0.000000
N	-2.978217	-2.006399	0.000000
H	-6.571726	0.716669	0.000000
N	-5.159768	-0.909539	0.000000
H	-5.768391	-1.715784	0.000000
H	5.669254	-1.963821	-0.871108

Supplementary information for

The effect of pi-stacking, h-bonding, and electrostatic interactions on the ionization energies of nucleobases: adenine-adenine, thymine-thymine and adenine-thymine dimers

Ksenia Bravaya[a], Oleg Kostko[b], Musahid Ahmed[b], and Anna I. Krylov[a]

[a] Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0482, USA

[b] Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Harmonic frequencies and thermodynamic analysis.

A. ωB97X-D/6-31+G(d,p), EML(75,302) grid

TT-HB1, C_2h

FREQUENCIES, cm-1

48.18	66.29	81.62
89.25	89.55	135.86
145.44	151.41	189.45
200.85	223.50	223.83
293.78	294.42	320.77
322.63	412.24	424.50
427.72	428.10	467.95
485.26	564.45	565.70
624.82	627.80	684.33
684.76	749.43	750.57
764.48	766.50	772.91
773.06	813.74	819.51
872.97	915.75	938.83
940.02	993.31	1002.08

1044.84	1045.68	1084.07
1084.10	1169.24	1169.38
1255.62	1257.22	1262.74
1263.51	1397.08	1399.22
1410.57	1410.65	1443.05
1443.12	1485.78	1485.79
1487.03	1495.29	1510.57
1510.67	1577.33	1583.93
1718.26	1718.47	1761.95
1765.98	1782.63	1792.49
3046.48	3046.63	3118.76
3118.76	3140.76	3140.76
3213.17	3247.54	3248.26
3268.00	3641.54	3641.64

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 147.012 kcal/mol

Translational Enthalpy:	0.889	kcal/mol
Rotational Enthalpy:	0.889	kcal/mol
Vibrational Enthalpy:	155.481	kcal/mol
gas constant (RT):	0.593	kcal/mol
Translational Entropy:	42.474	cal/mol.K
Rotational Entropy:	32.396	cal/mol.K
Vibrational Entropy:	53.045	cal/mol.K
Total Enthalpy:	157.851	kcal/mol
Total Entropy:	127.915	cal/mol.K

TT-HB1 cation, C_2h

FREQUENCIES, cm-1

-4853.26	22.41	41.42
77.34	86.58	101.66
113.70	128.50	143.18
155.18	156.10	167.07
180.30	293.25	295.31
317.66	318.92	402.37
403.69	409.61	419.95
461.68	509.09	561.10
561.27	615.02	616.00
685.62	685.80	739.77
740.45	742.25	743.18
746.32	758.52	807.99
823.26	869.38	899.76
949.28	958.89	991.31
991.53	1036.21	1038.77
1040.74	1040.95	1195.90
1196.03	1275.44	1279.43
1296.59	1300.51	1392.65
1410.16	1429.78	1431.05
1434.97	1435.82	1461.35
1461.50	1477.50	1492.19
1492.34	1530.24	1588.28
1612.04	1656.42	1735.03
1789.90	1824.71	1829.37
2731.59	3057.77	3059.17
3120.98	3121.02	3179.47
3184.47	3184.78	3257.04
3257.20	3631.51	3632.58

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

```
This Molecule has  1 Imaginary Frequencies
Zero point vibrational energy:      143.379 kcal/mol

Translational Enthalpy:        0.889 kcal/mol
Rotational Enthalpy:           0.889 kcal/mol
Vibrational Enthalpy:        152.206 kcal/mol
gas constant (RT):             0.593 kcal/mol
Translational Entropy:        42.474  cal/mol.K
Rotational Entropy:           32.366  cal/mol.K
Vibrational Entropy:          58.220  cal/mol.K

Total Enthalpy:              154.576 kcal/mol
Total Entropy:               133.061  cal/mol.K
```

TT-HB1 cation (HT), C_s

FREQUENCIES, cm-1

26.35	32.93	67.82
75.81	89.81	100.02
121.49	127.59	157.13
170.28	177.57	187.95
286.51	290.64	297.26
331.68	401.72	402.56
410.96	422.35	461.48
478.04	564.89	576.78
617.13	631.50	684.94
692.19	718.39	731.69
736.26	752.10	755.93
757.89	802.84	816.91
871.79	914.46	945.91
963.56	1011.77	1017.69

1019.67	1034.26	1070.14
1076.27	1144.84	1218.36
1241.70	1281.68	1289.08
1335.84	1381.27	1391.66
1408.83	1411.18	1434.24
1446.38	1448.27	1453.24
1478.28	1482.47	1500.36
1505.54	1539.56	1585.86
1638.55	1754.04	1758.36
1789.52	1799.60	1867.97
2632.06	3050.50	3077.22
3112.18	3152.98	3182.68
3183.43	3214.56	3270.13
3272.98	3623.63	3629.29

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 145.632 kcal/mol

Translational Enthalpy: 0.889 kcal/mol
Rotational Enthalpy: 0.889 kcal/mol
Vibrational Enthalpy: 154.528 kcal/mol
gas constant (RT): 0.593 kcal/mol
Translational Entropy: 42.474 cal/mol.K
Rotational Entropy: 33.720 cal/mol.K
Vibrational Entropy: 59.438 cal/mol.K

Total Enthalpy: 156.898 kcal/mol
Total Entropy: 135.632 cal/mol.K

TT-HB2, C_s

FREQUENCIES, cm-1

22.97	31.59	69.69
72.04	81.99	107.10
122.94	128.54	169.06
169.27	175.37	176.07
289.73	295.72	307.44
308.30	406.10	408.21
414.73	420.38	473.09
477.42	557.64	568.16
589.28	622.38	625.73
672.87	751.22	754.62
759.59	760.07	767.00
773.40	818.34	821.62
872.58	921.36	934.11
939.03	998.77	999.69
1037.37	1043.83	1075.76
1078.79	1189.10	1198.46
1251.31	1262.72	1268.98
1271.93	1393.26	1405.14
1421.60	1438.40	1439.47
1457.11	1484.04	1486.48
1495.90	1501.69	1505.23
1508.24	1551.96	1579.86
1738.40	1743.01	1761.91
1803.82	1820.72	1862.71
3065.45	3069.76	3141.76
3148.89	3154.77	3156.49
3241.08	3242.38	3279.65
3330.88	3658.42	3698.56

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 147.104 kcal/mol

Translational Enthalpy:	0.889	kcal/mol
Rotational Enthalpy:	0.889	kcal/mol
Vibrational Enthalpy:	156.013	kcal/mol
gas constant (RT):	0.593	kcal/mol
Translational Entropy:	42.474	cal/mol.K
Rotational Entropy:	33.828	cal/mol.K
Vibrational Entropy:	59.881	cal/mol.K
Total Enthalpy:	158.383	kcal/mol
Total Entropy:	136.183	cal/mol.K

TT-HB2 cation (HT), C_s

FREQUENCIES, cm-1

23.21	31.70	66.53
85.96	87.23	95.35
111.88	119.98	156.92
158.58	160.90	197.07
286.56	295.98	303.73
307.83	402.32	404.46
424.37	427.49	471.50
481.58	559.02	577.06
611.65	627.71	670.83
684.22	718.97	735.20
747.88	757.47	759.90
778.67	810.30	814.15
916.21	947.73	961.41
968.11	1000.33	1017.04

```
   1018.62                1037.42                1049.70
   1081.15                1215.72                1220.02
   1237.57                1278.43                1287.19
   1334.27                1373.61                1391.28
   1405.77                1413.01                1443.77
   1444.85                1453.69                1464.51
   1473.43                1492.42                1500.91
   1504.17                1518.86                1580.98
   1619.34                1681.93                1720.33
   1791.81                1803.69                1906.28
   2710.49                3053.18                3082.28
   3115.71                3164.03                3175.01
   3180.94                3210.69                3222.80
   3255.76                3623.45                3654.64

STANDARD THERMODYNAMIC QUANTITIES AT   298.18 K  AND     1.00 ATM

   This Molecule has  0 Imaginary Frequencies
   Zero point vibrational energy:      145.757 kcal/mol

   Translational Enthalpy:        0.889 kcal/mol
   Rotational Enthalpy:           0.889 kcal/mol
   Vibrational Enthalpy:        154.676 kcal/mol
   gas constant (RT):             0.593 kcal/mol
   Translational Entropy:        42.474  cal/mol.K
   Rotational Entropy:           33.763  cal/mol.K
   Vibrational Entropy:          60.119  cal/mol.K

   Total Enthalpy:              157.046 kcal/mol
   Total Entropy:               136.356  cal/mol.K
```

TT-HB3, C_s

FREQUENCIES, cm-1

17.18	39.15	62.08
63.00	76.93	118.86
119.78	136.73	164.64
165.02	172.54	174.73
284.74	285.65	298.82
304.20	404.73	406.21
413.24	421.63	474.08
474.85	557.57	559.10
567.30	620.95	621.58
677.20	751.10	753.20
753.37	758.21	765.37
771.13	818.98	823.32
854.38	910.83	922.02
937.66	999.07	1005.33
1043.11	1044.24	1074.09
1079.58	1179.71	1188.87
1236.28	1262.56	1269.18
1274.07	1405.28	1405.75
1421.40	1436.39	1441.28
1467.63	1481.02	1484.25
1493.66	1498.80	1504.32
1509.05	1534.53	1579.14
1743.03	1754.05	1794.71
1803.31	1820.19	1829.78
3065.26	3071.72	3136.92
3146.64	3160.99	3164.81
3243.36	3244.80	3299.10
3360.37	3660.43	3702.15

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

```
This Molecule has  0 Imaginary Frequencies
Zero point vibrational energy:      146.992 kcal/mol

Translational Enthalpy:        0.889 kcal/mol
Rotational Enthalpy:           0.889 kcal/mol
Vibrational Enthalpy:        155.966 kcal/mol
gas constant (RT):             0.593 kcal/mol
Translational Entropy:        42.474  cal/mol.K
Rotational Entropy:           33.737  cal/mol.K
Vibrational Entropy:          60.795  cal/mol.K

Total Enthalpy:              158.336 kcal/mol
Total Entropy:               137.006  cal/mol.K
```

TT-HB3 cation, C_s

18.49	31.64	55.62
65.30	91.21	101.58
119.67	125.26	132.51
154.71	158.95	164.79
285.85	290.23	298.24
312.96	393.00	404.57
407.42	426.82	457.57
474.39	545.13	567.99
591.40	606.34	631.40
675.82	714.69	728.50
736.12	749.10	751.62
760.62	774.00	792.70
828.46	906.40	929.31
934.80	1006.09	1008.57
1011.14	1057.24	1069.57
1158.72	1213.87	1217.12

```
    1226.10                1271.36                1275.54
    1338.55                1364.90                1400.77
    1404.52                1424.75                1438.11
    1441.15                1444.97                1453.06
    1476.81                1479.45                1492.81
    1501.10                1547.21                1560.42
    1654.88                1701.07                1750.69
    1805.36                1850.32                1853.53
    1973.08                3045.03                3082.62
    3103.63                3160.43                3181.03
    3189.60                3235.26                3268.15
    3540.53                3616.10                3683.34

 STANDARD THERMODYNAMIC QUANTITIES AT   298.18 K  AND     1.00 ATM

   This Molecule has  0 Imaginary Frequencies
   Zero point vibrational energy:      144.635 kcal/mol

   Translational Enthalpy:        0.889 kcal/mol
   Rotational Enthalpy:           0.889 kcal/mol
   Vibrational Enthalpy:        153.750 kcal/mol
   gas constant (RT):             0.593 kcal/mol
   Translational Entropy:        42.474  cal/mol.K
   Rotational Entropy:           33.707  cal/mol.K
   Vibrational Entropy:          62.334  cal/mol.K

   Total Enthalpy:              156.120 kcal/mol
   Total Entropy:               138.515  cal/mol.K
```

TT-HB3 cation (HT), C_s

```
FREQUENCIES, cm-1
```

19.09	36.02	63.52
71.07	86.28	100.24
124.26	127.85	149.58
160.72	168.17	173.92
282.94	288.91	294.60
320.24	399.83	401.83
411.44	421.92	472.69
477.16	548.79	574.83
604.81	614.79	627.02
689.25	718.72	733.58
735.91	753.91	755.52
756.29	806.06	818.48
897.20	911.45	948.16
961.94	1010.41	1018.96
1019.87	1069.05	1075.00
1075.72	1138.15	1220.57
1222.72	1276.27	1287.49
1335.76	1390.48	1402.73
1410.48	1418.64	1434.07
1443.39	1448.48	1454.09
1473.26	1477.72	1496.79
1501.24	1516.57	1584.31
1634.56	1748.00	1756.67
1793.78	1809.85	1870.52
2440.85	3051.45	3083.00
3111.76	3160.05	3186.77
3189.55	3210.85	3274.51
3282.66	3626.92	3669.20

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies

Zero point vibrational energy: 145.262 kcal/mol

Translational Enthalpy:	0.889	kcal/mol
Rotational Enthalpy:	0.889	kcal/mol
Vibrational Enthalpy:	154.257	kcal/mol
gas constant (RT):	0.593	kcal/mol
Translational Entropy:	42.474	cal/mol.K
Rotational Entropy:	33.671	cal/mol.K
Vibrational Entropy:	60.856	cal/mol.K
Total Enthalpy:	156.627	kcal/mol
Total Entropy:	137.002	cal/mol.K

TT-ST1, C_2

FREQUENCIES, cm-1

20.21	41.51	62.85
67.55	73.96	108.82
117.33	143.14	154.74
162.95	204.02	282.50
285.11	303.17	317.98
395.26	395.38	409.68
415.20	467.01	467.34
549.97	550.94	569.25
571.43	613.79	613.95
684.79	685.87	749.95
750.88	752.26	769.33
775.16	778.10	818.58
819.28	932.91	934.50
987.54	987.91	1033.01
1033.13	1074.24	1074.75
1185.93	1188.34	1233.74
1235.99	1264.23	1265.61

```
   1396.36              1397.26              1424.04
   1426.71              1433.95              1435.81
   1454.39              1457.36              1474.02
   1484.80              1497.73              1499.53
   1534.79              1542.19              1744.91
   1745.56              1788.23              1801.45
   1844.29              1856.55              3064.37
   3065.06              3136.18              3136.35
   3158.63              3158.92              3242.48
   3242.54              3641.57              3641.76
   3695.37              3695.40

  This Molecule has  0 Imaginary Frequencies

 STANDARD THERMODYNAMIC QUANTITIES AT   298.18 K  AND     1.00 ATM

  This Molecule has  0 Imaginary Frequencies
  Zero point vibrational energy:      146.531 kcal/mol

  Translational Enthalpy:        0.889 kcal/mol
  Rotational Enthalpy:           0.889 kcal/mol
  Vibrational Enthalpy:        155.243 kcal/mol
  gas constant (RT):             0.593 kcal/mol
  Translational Entropy:        42.474  cal/mol.K
  Rotational Entropy:           31.096  cal/mol.K
  Vibrational Entropy:          58.490  cal/mol.K

  Total Enthalpy:              157.614 kcal/mol
  Total Entropy:               132.060  cal/mol.K
```

TT-ST1 cation, C_1

```
FREQUENCIES, cm-1
```

30.73	49.65	50.54
75.75	91.16	108.74
135.88	137.60	141.22
147.49	162.67	187.64
286.43	292.11	295.59
309.65	389.94	396.76
401.33	403.65	461.36
462.00	535.66	547.75
601.56	603.04	663.40
666.97	681.30	687.58
718.93	734.83	740.01
752.92	763.12	763.60
799.76	802.85	952.96
958.32	961.40	967.25
1019.22	1019.72	1037.79
1040.92	1198.56	1205.79
1220.98	1245.77	1252.17
1285.20	1306.34	1374.03
1410.08	1424.40	1427.00
1436.53	1438.94	1442.27
1465.70	1479.21	1484.99
1494.49	1548.31	1562.11
1580.78	1661.73	1797.14
1801.48	1879.09	1888.34
3067.98	3072.45	3144.83
3146.72	3184.52	3193.08
3240.65	3248.97	3620.56
3626.30	3630.40	3637.91

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

```
This Molecule has  0 Imaginary Frequencies
Zero point vibrational energy:      146.052 kcal/mol


Translational Enthalpy:        0.889 kcal/mol
Rotational Enthalpy:           0.889 kcal/mol
Vibrational Enthalpy:        155.162 kcal/mol
gas constant (RT):             0.593 kcal/mol
Translational Entropy:        42.474  cal/mol.K
Rotational Entropy:           32.411  cal/mol.K
Vibrational Entropy:          60.010  cal/mol.K

Total Enthalpy:              157.532 kcal/mol
Total Entropy:               134.895  cal/mol.K
```

TT-ST1 cation, C_2

FREQUENCIES, cm-1

-32.38	-22.48	21.44
75.60	82.66	104.53
110.43	147.40	155.20
156.02	177.61	198.31
274.72	281.41	283.22
320.39	388.12	389.03
414.85	422.92	470.47
471.29	546.19	546.97
609.41	610.80	622.75
625.28	699.81	700.88
732.16	732.36	742.78
759.02	775.09	777.35
817.40	817.40	922.83
925.25	950.46	952.92
1016.46	1018.08	1065.47

1068.72	1205.98	1209.88
1234.24	1235.13	1289.40
1290.05	1356.42	1358.16
1425.16	1427.40	1435.81
1441.34	1444.15	1448.56
1480.06	1490.23	1511.10
1512.65	1566.42	1569.26
1675.36	1679.64	1814.44
1828.43	1907.14	1913.96
3059.55	3059.66	3128.89
3130.31	3176.14	3177.31
3239.34	3239.43	3617.91
3618.20	3633.25	3633.40

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 2 Imaginary Frequencies
Zero point vibrational energy: 146.453 kcal/mol

Translational Enthalpy: 0.889 kcal/mol
Rotational Enthalpy: 0.889 kcal/mol
Vibrational Enthalpy: 154.501 kcal/mol
gas constant (RT): 0.593 kcal/mol
Translational Entropy: 42.474 cal/mol.K
Rotational Entropy: 31.016 cal/mol.K
Vibrational Entropy: 51.071 cal/mol.K

Total Enthalpy: 156.871 kcal/mol
Total Entropy: 124.562 cal/mol.K

TT-ST3, C_1

FREQUENCIES, cm-1

24.40	43.16	52.32
71.80	84.28	98.20
128.85	135.23	153.35
167.13	177.41	191.38
284.30	284.34	313.27
318.54	395.95	396.39
407.07	413.59	467.20
467.93	549.44	553.03
559.33	580.01	613.28
614.38	677.48	700.73
747.96	750.05	760.67
768.41	774.79	780.91
817.16	819.92	915.34
938.51	988.28	990.35
1033.79	1038.68	1073.97
1080.39	1179.98	1188.48
1225.57	1237.29	1261.80
1265.89	1398.30	1398.57
1424.34	1430.12	1432.97
1434.96	1455.95	1458.08
1480.20	1481.85	1501.38
1505.23	1529.42	1538.82
1744.04	1744.44	1799.50
1811.77	1836.41	1849.29
3068.16	3068.40	3143.59
3150.56	3157.45	3165.00
3237.54	3252.20	3637.44
3648.04	3686.61	3705.69

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 146.872 kcal/mol

Translational Enthalpy: 0.889 kcal/mol
Rotational Enthalpy: 0.889 kcal/mol
Vibrational Enthalpy: 155.954 kcal/mol
gas constant (RT): 0.593 kcal/mol
Translational Entropy: 42.474 cal/mol.K
Rotational Entropy: 32.504 cal/mol.K
Vibrational Entropy: 60.527 cal/mol.K

Total Enthalpy: 158.324 kcal/mol
Total Entropy: 135.506 cal/mol.K

TT-ST3 cation, C_1

FREQUENCIES, cm-1

18.13	25.89	43.60
49.40	55.51	81.81
90.89	109.41	119.68
130.09	167.98	211.88
288.82	290.95	298.05
306.06	375.54	391.61
398.14	417.37	454.05
470.76	539.73	556.77
595.25	613.55	643.35
666.57	681.83	701.74
722.57	732.34	754.84
762.95	766.21	782.84
790.96	813.72	940.55
948.59	957.44	981.03
1004.22	1014.60	1024.47

1069.31	1203.60	1210.17
1237.52	1249.67	1250.53
1293.71	1337.01	1371.05
1391.33	1418.89	1425.68
1435.53	1444.36	1452.35
1461.49	1479.44	1486.95
1497.83	1553.18	1558.98
1616.69	1687.51	1706.91
1828.16	1884.09	1892.76
3053.33	3075.43	3126.42
3144.33	3178.12	3195.64
3249.73	3249.99	3613.48
3616.24	3630.65	3665.40

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 145.867 kcal/mol

Translational Enthalpy: 0.889 kcal/mol
Rotational Enthalpy: 0.889 kcal/mol
Vibrational Enthalpy: 155.237 kcal/mol
gas constant (RT): 0.593 kcal/mol
Translational Entropy: 42.474 cal/mol.K
Rotational Entropy: 32.654 cal/mol.K
Vibrational Entropy: 66.475 cal/mol.K

Total Enthalpy: 157.607 kcal/mol
Total Entropy: 141.604 cal/mol.K

AA-HB1, C_2h

FREQUENCIES, cm-1

27.43	33.19	74.28
76.25	93.62	114.15
159.16	163.97	187.13
191.87	228.91	234.30
282.87	287.14	310.62
315.66	531.52	541.69
544.00	548.83	549.70
549.71	571.75	573.33
622.77	625.37	665.26
667.86	699.21	699.26
740.66	742.15	813.82
814.03	894.06	894.20
911.67	918.78	929.81
931.99	956.72	956.75
990.74	990.94	1024.56
1025.45	1155.10	1159.59
1197.23	1199.62	1268.63
1268.75	1304.79	1317.63
1364.92	1366.95	1398.22
1401.03	1422.23	1422.47
1482.19	1485.02	1514.28
1518.53	1544.45	1554.91
1558.88	1561.89	1641.09
1644.46	1683.62	1692.62
1696.17	1707.16	3163.73
3203.34	3208.51	3215.36
3288.50	3288.56	3658.08
3658.31	3803.08	3803.11

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 143.715 kcal/mol

Translational Enthalpy:	0.889	kcal/mol
Rotational Enthalpy:	0.889	kcal/mol
Vibrational Enthalpy:	152.045	kcal/mol
gas constant (RT):	0.593	kcal/mol
Translational Entropy:	42.680	cal/mol.K
Rotational Entropy:	32.605	cal/mol.K
Vibrational Entropy:	54.691	cal/mol.K
Total Enthalpy:	154.415	kcal/mol
Total Entropy:	129.976	cal/mol.K

AA-HB1 cation, C_2

FREQUENCIES, cm-1

27.71	32.40	73.57
95.29	97.32	112.44
156.10	168.83	222.55
226.34	285.35	293.75
296.89	303.10	520.81
526.61	529.56	531.25
535.27	538.78	539.49
551.37	593.90	594.90
616.60	625.33	626.77
636.51	693.95	694.08
745.30	767.24	803.41
803.49	902.42	912.39
914.75	921.57	924.69
931.19	942.24	978.65
996.12	996.49	1021.78

1022.91	1165.29	1165.42
1192.32	1202.68	1255.81
1255.96	1278.92	1307.27
1362.44	1369.91	1422.90
1426.28	1433.73	1436.14
1451.03	1470.73	1515.02
1518.33	1533.28	1538.36
1552.23	1619.19	1635.51
1635.79	1681.25	1693.43
1696.60	2416.13	3167.62
3229.24	3229.98	3296.93
3297.10	3588.13	3614.35
3754.79	3754.79	5811.55

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 149.116 kcal/mol

Translational Enthalpy:	0.889	kcal/mol
Rotational Enthalpy:	0.889	kcal/mol
Vibrational Enthalpy:	156.998	kcal/mol
gas constant (RT):	0.593	kcal/mol
Translational Entropy:	42.680	cal/mol.K
Rotational Entropy:	32.606	cal/mol.K
Vibrational Entropy:	51.268	cal/mol.K
Total Enthalpy:	159.369	kcal/mol
Total Entropy:	126.554	cal/mol.K

AA-HB1 cation (HT), C_s

FREQUENCIES, cm-1

27.12	35.85	70.86
77.80	85.58	128.51
150.47	171.23	209.43
223.68	285.32	285.74
291.93	313.74	485.40
492.21	522.04	524.19
536.32	540.73	553.71
564.09	587.96	605.40
617.93	620.22	626.13
658.71	688.11	704.07
735.80	748.93	779.41
794.52	882.92	900.83
901.12	913.21	945.83
957.11	957.65	963.72
997.62	1014.82	1015.93
1019.80	1114.78	1143.37
1162.33	1178.79	1228.69
1247.38	1283.72	1318.03
1327.81	1357.65	1401.21
1407.34	1425.73	1455.07
1471.98	1487.21	1506.26
1527.73	1544.88	1556.83
1565.62	1631.55	1637.56
1669.88	1678.67	1702.12
1722.99	1728.24	3029.26
3229.16	3246.94	3257.92
3275.29	3298.82	3602.81
3628.65	3743.19	3768.60

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies

Zero point vibrational energy: 144.069 kcal/mol

Translational Enthalpy:	0.889	kcal/mol
Rotational Enthalpy:	0.889	kcal/mol
Vibrational Enthalpy:	152.028	kcal/mol
gas constant (RT):	0.593	kcal/mol
Translational Entropy:	42.680	cal/mol.K
Rotational Entropy:	33.980	cal/mol.K
Vibrational Entropy:	51.962	cal/mol.K
Total Enthalpy:	154.399	kcal/mol
Total Entropy:	128.622	cal/mol.K

AA-ST, C_1

FREQUENCIES, cm-1

24.97	32.55	43.48
73.64	87.99	97.71
174.99	182.78	220.01
229.10	283.48	286.88
309.19	312.18	461.25
474.84	490.01	503.86
529.49	533.39	535.88
539.11	542.55	547.34
580.92	586.27	627.44
628.51	670.96	673.71
699.19	702.95	738.19
738.96	819.64	821.97
878.89	885.71	912.77
913.53	953.82	955.38
994.56	997.76	1050.16

1050.93	1114.27	1115.08
1171.51	1172.50	1275.21
1276.46	1289.78	1290.62
1364.41	1366.06	1390.52
1391.46	1404.14	1405.36
1449.77	1452.80	1477.09
1479.40	1539.44	1541.90
1566.57	1568.42	1639.75
1644.73	1683.44	1686.40
1695.90	1699.62	3206.35
3217.94	3291.19	3296.15
3631.49	3641.53	3719.52
3720.60	3763.86	3775.13

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 144.123 kcal/mol

Translational Enthalpy:	0.889	kcal/mol
Rotational Enthalpy:	0.889	kcal/mol
Vibrational Enthalpy:	152.327	kcal/mol
gas constant (RT):	0.593	kcal/mol
Translational Entropy:	42.680	cal/mol.K
Rotational Entropy:	32.846	cal/mol.K
Vibrational Entropy:	54.368	cal/mol.K
Total Enthalpy:	154.698	kcal/mol
Total Entropy:	129.895	cal/mol.K

AA-ST cation, C_1

FREQUENCIES, cm-1

38.05	61.64	73.07
99.90	110.48	140.37
179.49	190.46	235.06
239.41	285.31	287.50
306.81	313.40	405.19
482.79	524.08	525.77
528.72	531.14	537.58
544.48	571.66	586.13
598.65	612.28	618.12
621.35	645.89	649.27
691.40	695.15	738.25
743.54	809.29	813.27
904.75	906.47	921.43
924.85	935.14	942.34
1000.44	1012.73	1025.54
1034.51	1094.42	1126.17
1143.22	1163.71	1230.46
1267.01	1270.50	1275.62
1344.88	1362.19	1365.83
1413.30	1418.26	1426.04
1438.85	1447.23	1456.81
1461.07	1489.45	1523.75
1533.22	1537.54	1615.87
1624.03	1650.95	1680.65
1682.38	1694.68	3229.54
3236.19	3292.19	3297.05
3603.89	3614.05	3692.53
3692.93	3750.48	3756.17

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 143.738 kcal/mol

Translational Enthalpy:	0.889	kcal/mol
Rotational Enthalpy:	0.889	kcal/mol
Vibrational Enthalpy:	151.692	kcal/mol
gas constant (RT):	0.593	kcal/mol
Translational Entropy:	42.680	cal/mol.K
Rotational Entropy:	32.658	cal/mol.K
Vibrational Entropy:	49.117	cal/mol.K
Total Enthalpy:	154.062	kcal/mol
Total Entropy:	124.455	cal/mol.K

AT-HB1, C_1

FREQUENCIES, cm-1

16.89	33.46	68.22
69.86	86.46	117.44
127.29	137.57	158.80
171.31	185.08	233.37
283.64	285.71	302.25
312.86	409.74	412.36
474.76	537.79	543.65
551.84	566.48	572.43
622.93	626.36	665.87
681.12	698.56	740.59
755.56	761.57	767.88
813.79	820.54	858.27
894.38	921.89	926.85
939.96	959.47	992.56
997.76	1028.92	1040.03

1074.61	1145.20	1187.95
1191.01	1267.48	1269.56
1273.08	1300.92	1366.12
1400.09	1406.98	1420.53
1423.29	1437.80	1480.19
1483.42	1491.64	1501.06
1508.59	1544.01	1557.39
1608.51	1644.24	1684.28
1700.90	1745.63	1800.93
1815.23	3070.63	3142.68
3158.17	3166.50	3216.63
3247.97	3301.52	3386.33
3658.26	3658.48	3804.01

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 145.410 kcal/mol

Translational Enthalpy:	0.889	kcal/mol
Rotational Enthalpy:	0.889	kcal/mol
Vibrational Enthalpy:	154.087	kcal/mol
gas constant (RT):	0.593	kcal/mol
Translational Entropy:	42.579	cal/mol.K
Rotational Entropy:	33.931	cal/mol.K
Vibrational Entropy:	58.645	cal/mol.K
Total Enthalpy:	156.457	kcal/mol
Total Entropy:	135.155	cal/mol.K

AT-HB1 cation, C_1

FREQUENCIES, cm-1

10.76	35.52	37.61
67.87	87.13	117.49
143.27	148.23	149.16
178.06	223.41	281.88
283.98	288.45	309.75
405.85	421.78	474.67
481.53	515.25	546.81
561.37	564.64	610.54
620.09	626.07	641.22
668.28	710.58	715.98
741.34	749.14	756.75
766.24	798.28	821.34
899.60	911.72	911.82
951.66	992.37	1003.01
1014.97	1047.86	1070.54
1099.95	1129.60	1169.45
1195.92	1208.56	1243.29
1260.91	1273.33	1337.01
1412.11	1412.73	1417.88
1437.83	1450.12	1475.33
1478.48	1490.85	1502.13
1510.26	1535.95	1549.15
1569.01	1627.03	1697.78
1711.16	1751.28	1764.34
1848.33	2454.98	3080.22
3155.86	3180.97	3254.90
3255.24	3302.86	3550.22
3584.87	3643.45	3724.37

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 144.546 kcal/mol

Translational Enthalpy: 0.889 kcal/mol
Rotational Enthalpy: 0.889 kcal/mol
Vibrational Enthalpy: 153.079 kcal/mol
gas constant (RT): 0.593 kcal/mol
Translational Entropy: 42.579 cal/mol.K
Rotational Entropy: 33.966 cal/mol.K
Vibrational Entropy: 59.057 cal/mol.K

Total Enthalpy: 155.449 kcal/mol
Total Entropy: 135.602 cal/mol.K

AT-HB1 cation (HT), C_s

FREQUENCIES, cm-1

20.00	27.57	53.19
54.27	63.82	76.38
104.76	126.74	152.95
169.44	205.11	278.09
283.35	291.21	313.09
401.06	411.28	465.74
497.25	519.79	533.40
539.59	572.29	609.54
616.99	619.61	655.16
686.18	687.42	721.76
732.69	735.92	763.94
772.15	779.14	812.26
902.87	916.49	923.93
949.08	953.03	961.75

```
     994.70                1011.18                1017.73
    1019.78                1112.64                1176.42
    1219.88                1242.16                1276.28
    1283.39                1333.02                1345.70
    1389.10                1402.15                1408.03
    1430.67                1439.66                1451.75
    1460.02                1463.40                1500.18
    1525.89                1559.98                1565.59
    1571.13                1618.19                1672.76
    1717.49                1726.85                1788.98
    1799.20                3057.86                3118.24
    3159.02                3192.46                3194.22
    3242.96                3310.60                3552.17
    3626.08                3628.08                3765.55

STANDARD THERMODYNAMIC QUANTITIES AT   298.18 K  AND     1.00 ATM

  This Molecule has  0 Imaginary Frequencies
  Zero point vibrational energy:      144.861 kcal/mol

  Translational Enthalpy:        0.889 kcal/mol
  Rotational Enthalpy:           0.889 kcal/mol
  Vibrational Enthalpy:        153.594 kcal/mol
  gas constant (RT):             0.593 kcal/mol
  Translational Entropy:        42.579  cal/mol.K
  Rotational Entropy:           33.952  cal/mol.K
  Vibrational Entropy:          60.818  cal/mol.K

  Total Enthalpy:              155.965 kcal/mol
  Total Entropy:               137.349  cal/mol.K
```

AT-HB2, C_1

FREQUENCIES, cm-1

13.91	23.42	59.47
62.59	95.16	116.62
118.35	146.08	166.95
169.90	226.63	283.77
301.85	304.65	319.94
407.61	411.79	473.10
474.00	537.77	542.20
542.83	567.80	583.57
622.78	643.61	670.64
676.41	697.61	741.09
754.39	755.33	766.71
768.03	811.90	819.60
875.91	922.16	922.96
937.85	955.45	983.42
995.62	1040.87	1057.06
1076.60	1107.91	1179.17
1191.64	1266.64	1269.12
1281.85	1289.43	1378.77
1398.50	1405.90	1406.69
1421.45	1438.31	1451.51
1482.70	1489.04	1500.28
1509.12	1555.33	1567.17
1613.07	1666.63	1681.27
1718.58	1741.77	1805.01
1819.51	3069.66	3140.56
3144.73	3161.09	3207.23
3246.46	3291.44	3420.70
3663.35	3718.18	3733.70

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 145.644 kcal/mol

Translational Enthalpy: 0.889 kcal/mol
Rotational Enthalpy: 0.889 kcal/mol
Vibrational Enthalpy: 154.135 kcal/mol
gas constant (RT): 0.593 kcal/mol
Translational Entropy: 42.579 cal/mol.K
Rotational Entropy: 33.940 cal/mol.K
Vibrational Entropy: 58.446 cal/mol.K

Total Enthalpy: 156.505 kcal/mol
Total Entropy: 134.965 cal/mol.K

AT-HB2 cation, C_1

FREQUENCIES, cm-1

14.26	31.43	51.74
69.70	97.73	114.19
138.32	142.64	156.57
177.48	234.22	279.01
284.30	308.07	341.43
403.52	423.39	480.27
481.62	527.04	543.99
566.08	571.76	621.19
640.87	643.65	662.35
675.43	725.35	743.89
747.32	750.66	758.53
770.78	797.12	822.20
901.82	909.75	931.79
932.01	1002.61	1010.94

1049.24	1059.64	1070.11
1110.39	1131.46	1148.75
1171.06	1237.69	1246.59
1254.68	1272.42	1345.82
1411.61	1418.41	1427.34
1437.96	1448.00	1458.48
1476.23	1478.11	1489.72
1501.84	1515.09	1550.50
1566.96	1603.03	1677.37
1710.39	1751.20	1766.65
1846.73	2469.85	3080.07
3155.27	3180.60	3238.88
3256.35	3307.61	3528.77
3622.27	3642.24	3679.00

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 144.789 kcal/mol

Translational Enthalpy:	0.889	kcal/mol
Rotational Enthalpy:	0.889	kcal/mol
Vibrational Enthalpy:	153.198	kcal/mol
gas constant (RT):	0.593	kcal/mol
Translational Entropy:	42.579	cal/mol.K
Rotational Entropy:	33.964	cal/mol.K
Vibrational Entropy:	57.355	cal/mol.K
Total Enthalpy:	155.568	kcal/mol
Total Entropy:	133.898	cal/mol.K

AT-HB2 cation (HT), C_1

FREQUENCIES, cm-1

16.65	26.38	53.26
59.95	72.06	91.20
125.77	127.73	153.28
174.54	232.25	282.27
288.02	294.55	305.34
397.35	416.31	465.80
526.27	537.97	561.74
564.83	572.82	619.42
628.39	630.82	664.04
685.92	689.54	720.80
735.73	738.31	753.03
764.53	788.01	811.48
909.75	914.33	920.46
946.18	955.03	956.85
968.88	1013.26	1018.40
1050.69	1109.85	1178.03
1221.08	1231.64	1284.42
1287.46	1333.42	1371.21
1389.88	1397.07	1410.78
1438.71	1441.80	1456.24
1465.16	1482.66	1501.47
1502.45	1518.28	1567.20
1568.88	1649.84	1668.39
1699.31	1759.14	1789.29
1802.22	3054.00	3120.73
3184.43	3204.12	3229.74
3258.33	3298.68	3431.09
3624.77	3687.98	3704.67

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND 1.00 ATM

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 145.180 kcal/mol

Translational Enthalpy: 0.889 kcal/mol
Rotational Enthalpy: 0.889 kcal/mol
Vibrational Enthalpy: 153.767 kcal/mol
gas constant (RT): 0.593 kcal/mol
Translational Entropy: 42.579 cal/mol.K
Rotational Entropy: 33.940 cal/mol.K
Vibrational Entropy: 59.511 cal/mol.K

Total Enthalpy: 156.137 kcal/mol
Total Entropy: 136.029 cal/mol.K

AT-ST1, C_1

FREQUENCIES, cm-1

-54.58	26.21	31.30
53.62	82.98	107.82
114.09	132.27	166.05
196.82	222.45	282.55
287.05	304.60	314.48
394.69	402.29	468.48
487.43	503.96	518.99
534.01	545.93	554.49
565.54	577.81	615.09
627.90	659.84	675.32
697.99	738.30	750.08
759.62	773.89	816.36
818.98	888.23	913.06
918.53	954.66	986.60

```
     991.10                1035.66                1052.91
    1077.18                1115.97                1170.22
    1184.68                1232.46                1266.56
    1275.96                1291.51                1363.05
    1392.49                1399.46                1404.64
    1423.37                1433.88                1449.88
    1458.83                1477.10                1482.19
    1497.78                1535.57                1542.90
    1567.83                1644.30                1682.91
    1696.54                1746.18                1801.92
    1833.55                3067.52                3144.86
    3161.67                3217.23                3249.06
    3295.21                3631.94                3660.70
    3700.71                3718.90                3762.47

STANDARD THERMODYNAMIC QUANTITIES AT   298.18 K  AND     1.00 ATM

  This Molecule has  1 Imaginary Frequencies
  Zero point vibrational energy:      145.258 kcal/mol

  Translational Enthalpy:        0.889 kcal/mol
  Rotational Enthalpy:           0.889 kcal/mol
  Vibrational Enthalpy:        153.469 kcal/mol
  gas constant (RT):             0.593 kcal/mol
  Translational Entropy:        42.579  cal/mol.K
  Rotational Entropy:           32.586  cal/mol.K
  Vibrational Entropy:          54.035  cal/mol.K

  Total Enthalpy:              155.840 kcal/mol
  Total Entropy:               129.200  cal/mol.K
```

B. B3LYP-D/6-31+G(d,p), EML(75,302) grid

AT-ST1, C_1

FREQUENCIES, cm-1

30.74	36.51	60.86
79.98	111.77	118.27
146.42	154.41	172.16
200.17	229.92	282.86
287.78	312.25	314.59
390.97	404.59	459.17
464.07	511.56	521.50
530.18	540.97	552.43
558.76	577.57	608.63
620.53	650.03	664.80
690.48	726.90	739.05
748.53	761.57	805.82
807.64	859.54	900.41
905.89	941.44	973.03
976.30	1028.71	1045.89
1072.18	1084.87	1149.05
1156.95	1201.20	1235.80
1258.90	1267.81	1336.25
1366.12	1371.59	1375.94
1411.68	1422.84	1423.61
1428.27	1440.67	1467.40
1484.17	1500.76	1510.99
1524.12	1618.55	1640.59
1670.98	1699.60	1749.41
1786.25	3023.07	3100.75
3112.05	3176.07	3219.32
3261.66	3566.99	3610.10

```
     3652.04                3658.37                3697.36

STANDARD THERMODYNAMIC QUANTITIES AT   298.18 K  AND     1.00 ATM

  This Molecule has  0 Imaginary Frequencies
  Zero point vibrational energy:      143.300 kcal/mol

  Translational Enthalpy:        0.889 kcal/mol
  Rotational Enthalpy:           0.889 kcal/mol
  Vibrational Enthalpy:        151.917 kcal/mol
  gas constant (RT):             0.593 kcal/mol
  Translational Entropy:        42.579  cal/mol.K
  Rotational Entropy:           32.505  cal/mol.K
  Vibrational Entropy:          55.657  cal/mol.K

  Total Enthalpy:              154.287 kcal/mol
  Total Entropy:               130.741  cal/mol.K
```