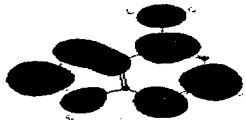
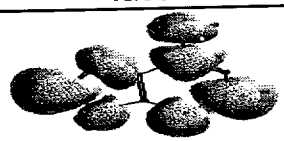
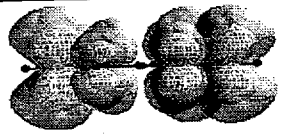
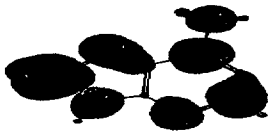
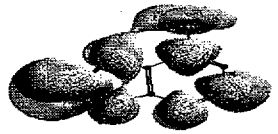
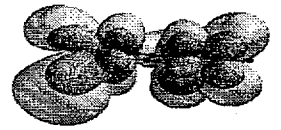
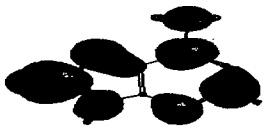
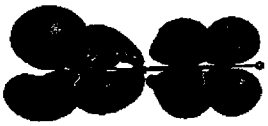
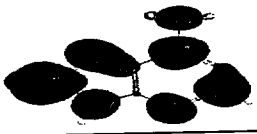
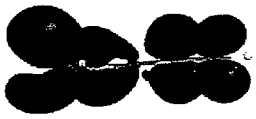
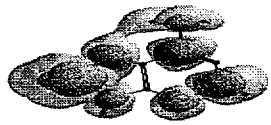
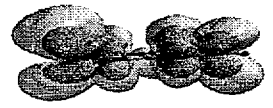
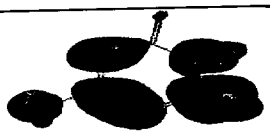
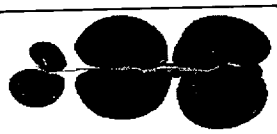
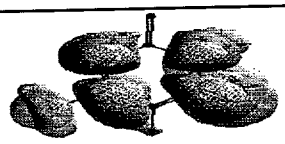
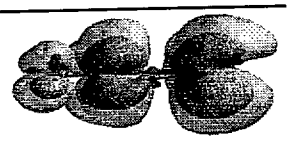
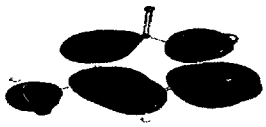
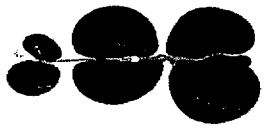
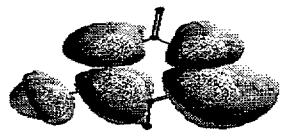
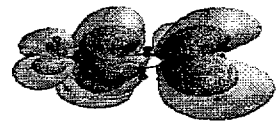
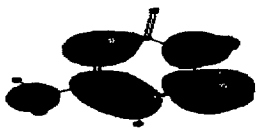
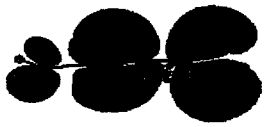
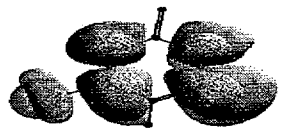
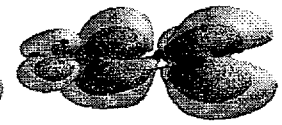
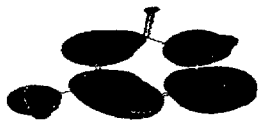
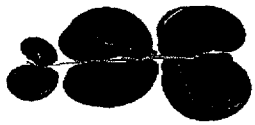
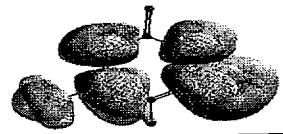
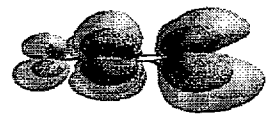
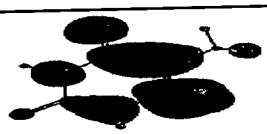
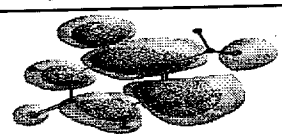
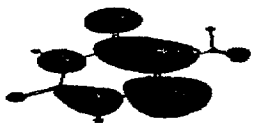
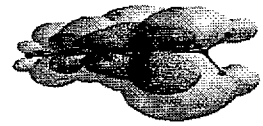
Supporting information for "DFT Calculations of the Electron Affinities ..."

By Xifeng Li, Zhongli Cai and Michael Sevilla

Base	SOMO face	SOMO edge	B3LYP / basis set	SPIN face	SPIN edge
A			6-31G(D)		
A			6-31+G(D)		
A			D95V(D)		
A			D95V+(D)		
C			6-31G(D)		
C			6-31+G(D)		
C			D95V(D)		
C			D95V+(D)		
T			6-31G(D)		
T			6-31+G(D)		
T			D95V(D)		
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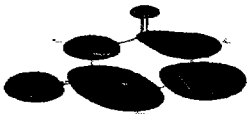
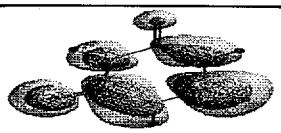
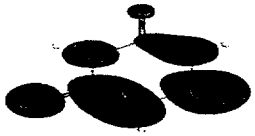
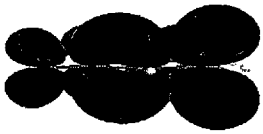
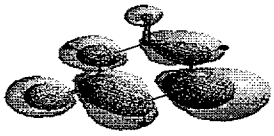
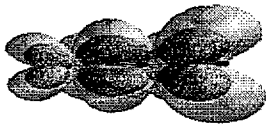
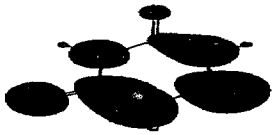
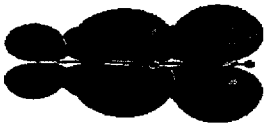
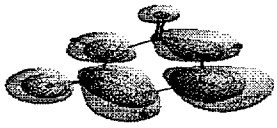
U			6-31G(D)		
U			6-31+G(D)		
U			D95V(D)		
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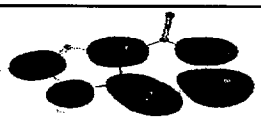
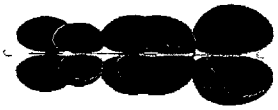
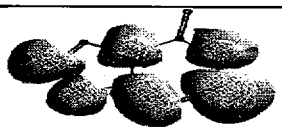
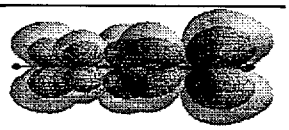
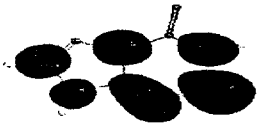
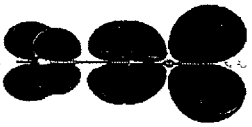
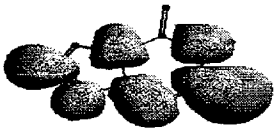
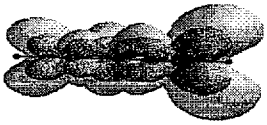
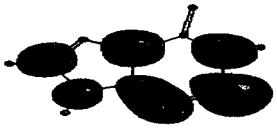
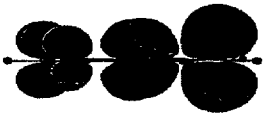
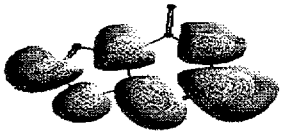
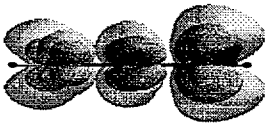
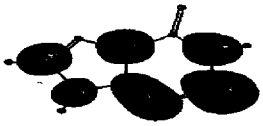
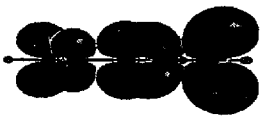
I			6-31G(D)		
I			6-31+G(D)		
I			D95V(D)		
I			D95V+(D)		

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B3LYP Calculated Dipole moments of neutral bases (Debye)

base	G	A	C	T	U	I
6-31G(D)	6.84	2.37	6.38	4.20	4.26	5.06
6-31+G(D)	7.10	2.47	6.91	4.69	4.67	5.44
6-311++G(2d,p)	6.96	2.41	6.70	4.51	4.52	5.31
D95V(D)	7.05	2.43	6.68	4.48	4.48	5.26
D95V+(D)	7.08	2.46	6.89	4.67	4.65	5.41

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Structures of DNA/RNA bases optimized at B3LYP/D95V+(D) level

Bases: guanine, adenine, cytosine, thymine, uracil, hypoxanthine.

Charge: anion(-1), neutral (0), cation (+1).

----------guanine

----------guanine anion----------

-1 2

1	-2.016399	0.000000	-3.292097
7	-2.031270	0.000000	-1.157079
6	-0.913991	0.000000	1.169670
6	0.261179	0.000000	-0.968339
8	-1.835080	0.000000	1.985881
6	-0.957647	0.000000	-0.274547
7	0.437948	0.000000	1.619421
7	-0.094298	0.000000	-2.300124
1	0.555777	0.000000	2.637900
7	1.525198	0.000000	-0.494082
1	2.842946	0.000000	2.491914
6	-1.480428	0.000000	-2.348021
1	0.556063	0.000000	-3.079741
6	1.573722	0.000000	0.835125
7	2.766323	0.000000	1.469245
1	3.617937	0.000000	0.909987

----------guanine neutral----------

0 1

1	-2.014154	0.000000	-3.291427
7	-2.027886	0.000000	-1.158705
6	-0.929037	0.000000	1.164124
6	0.259847	0.000000	-0.971364
8	-1.830452	0.000000	1.990664
6	-0.958144	0.000000	-0.278883
7	0.436325	0.000000	1.620719
7	-0.089897	0.000000	-2.299742
1	0.515463	0.000000	2.634828
7	1.528016	0.000000	-0.481855
1	2.871626	0.000000	2.474319
6	-1.477720	0.000000	-2.348450
1	0.557384	0.000000	-3.080075
6	1.563242	0.000000	0.834159
7	2.775894	0.000000	1.469091
1	3.607010	0.000000	0.892959

----------guanine cation----------

1 2

1	-1.998645	0.000000	-3.282215
7	-2.002767	0.000000	-1.132105
6	-0.934922	0.000000	1.182909
6	0.293976	0.000000	-0.988938
8	-1.855066	0.000000	1.965524
6	-0.966706	0.000000	-0.283195
7	0.425928	0.000000	1.653752
7	-0.069909	0.000000	-2.317632

1	0.502282	0.000000	2.671746
7	1.509392	0.000000	-0.484779
1	2.907484	0.000000	2.443727
6	-1.440465	0.000000	-2.350663
1	0.563607	0.000000	-3.114827
6	1.544064	0.000000	0.876569
7	2.755064	0.000000	1.439540
1	3.566170	0.000000	0.825857

----------adenine

----------adenine anion----------

-1 2

1	2.742811	1.025737	-0.121712
7	2.014900	1.688423	-0.391867
7	1.305405	-1.327237	-0.316618
7	-0.829629	-2.003894	0.139419
6	0.476682	-2.418288	-0.292199
1	0.837138	-3.403055	0.014921
1	-2.311033	2.234206	0.516766
1	2.141006	2.583002	0.081827
1	-1.674630	-2.551289	0.032347
7	-0.291194	2.008805	0.125742
6	-1.512565	1.508929	0.343848
7	-1.888207	0.188947	0.368517
6	-0.845609	-0.627835	0.160067
6	0.499799	-0.248660	-0.101192
6	0.729323	1.156870	-0.110607

----------adenine neutral----------

0 1

1	2.794917	1.039805	-0.321066
7	2.005258	1.657186	-0.186303
7	1.310011	-1.349722	-0.239340
7	-0.835964	-1.995181	0.014579
6	0.481797	-2.368991	-0.178600
1	0.768750	-3.411835	-0.267170
1	-2.310439	2.221619	0.414446
1	2.138486	2.659815	-0.155492
1	-1.644007	-2.602559	0.092569
7	-0.278848	1.999559	0.133760
6	-1.515819	1.487545	0.273363
7	-1.899275	0.204232	0.262245
6	-0.851736	-0.615230	0.083420
6	0.491288	-0.240537	-0.076914
6	0.751808	1.150652	-0.044248

----------adenine cation----------

1 2

1	2.798737	1.056349	-0.320817
7	1.990605	1.662203	-0.184106
7	1.301443	-1.330587	-0.237358
7	-0.844268	-2.016497	0.014609
6	0.450665	-2.377059	-0.174753
1	0.760760	-3.413922	-0.266122
1	-2.300960	2.227592	0.413516
1	2.120248	2.674110	-0.152392
1	-1.649444	-2.636144	0.091579
7	-0.275803	2.015340	0.134145
6	-1.489526	1.514766	0.271177
7	-1.876929	0.185472	0.258366
6	-0.868913	-0.627514	0.085094
6	0.509207	-0.257214	-0.080102

6	0.766120	1.160438	-0.045643

----------cytosine

----------cytosine anion----------

-1 2

6	1.396227	0.000000	-1.127981
1	1.399521	0.000000	2.972991
1	2.576559	0.000000	0.707858
1	-0.178131	0.000000	-2.557111
1	2.185384	0.000000	-1.873479
7	0.516893	0.000000	2.485659
1	-0.351656	0.000000	3.000323
6	1.573340	0.000000	0.278336
7	0.054432	0.000000	-1.572630
6	-1.070000	0.000000	-0.714050
8	-2.197265	0.000000	-1.265361
7	-0.865375	0.000000	0.625529
6	0.434566	0.000000	1.080761

----------cytosine neutral----------

0 1

6	1.352666	0.000000	-1.080695
1	1.432580	0.000000	2.899494
1	2.572386	0.000000	0.680465
1	-0.108051	0.000000	-2.561754
1	2.159949	0.000000	-1.810747
7	0.525934	0.000000	2.454154
1	-0.311304	0.000000	3.024529
6	1.568257	0.000000	0.267178
7	0.083727	0.000000	-1.564694
6	-1.076365	0.000000	-0.729141
8	-2.176495	0.000000	-1.269442
7	-0.852669	0.000000	0.624441
6	0.383351	0.000000	1.097033

----------cytosine cation----------

1 2

6	1.335149	0.000000	-1.113913
1	1.411531	0.000000	2.931915
1	2.561998	0.000000	0.652896
1	-0.122526	0.000000	-2.588480
1	2.153452	0.000000	-1.831371
7	0.512303	0.000000	2.462162
1	-0.331565	0.000000	3.030835
6	1.546981	0.000000	0.263501
7	0.084408	0.000000	-1.587058
6	-1.039282	0.000000	-0.715099
8	-2.159840	0.000000	-1.257115
7	-0.856809	0.000000	0.621389
6	0.394905	0.000000	1.129789

----------thymine

----------thymine anion----------

-1 2

6	-1.609680	-0.405598	-0.233412
1	2.670906	2.002627	-0.444505
8	-2.743132	-0.901256	-0.408115
1	-0.113420	2.634007	0.112325
1	3.130418	0.525527	0.441367
8	1.784944	-1.584305	0.160530
6	1.021250	0.717433	0.170397

1	-2.235884	1.502483	-0.224433
6	-0.123666	1.550055	0.058533
6	2.382341	1.324248	0.380597
6	0.895846	-0.685426	0.085853
1	-0.576737	-2.166526	-0.181459
7	-1.398282	0.942135	-0.140213
7	-0.465106	-1.161497	-0.117971
1	2.437399	1.917635	1.312865

----------thymine neutral----------

0	1		
6	-1.613537	-0.419916	-0.234732
1	2.668152	1.996909	-0.445715
8	-2.726820	-0.895643	-0.405655
1	-0.103418	2.583015	0.111218
1	3.113575	0.525829	0.439174
8	1.780615	-1.530227	0.162543
6	1.003998	0.745724	0.169488
1	-2.201076	1.532106	-0.218337
6	-0.123191	1.495861	0.056004
6	2.379135	1.334225	0.380649
6	0.864338	-0.719137	0.080120
1	-0.577660	-2.180928	-0.182260
7	-1.377045	0.946503	-0.137180
7	-0.455654	-1.172567	-0.117259
1	2.434497	1.911934	1.312715

----------thymine cation----------

1	2		
6	-1.598803	-0.449817	-0.234265
1	2.612000	2.003874	-0.444245
8	-2.725412	-0.838193	-0.402683
1	-0.107313	2.615786	0.112299
1	3.118012	0.530274	0.439948
8	1.791196	-1.524112	0.164261
6	1.013370	0.728467	0.169893
1	-2.188937	1.544525	-0.216125
6	-0.149925	1.527988	0.054012
6	2.358626	1.312438	0.376866
6	0.853936	-0.757110	0.076920
1	-0.588481	-2.223564	-0.185740
7	-1.342363	0.973366	-0.131274
7	-0.459835	-1.211069	-0.119678
1	2.380602	1.919676	1.297346

----------uracil

----------uracil anion----------

-1	2		
8	-1.052504	0.000000	-2.341353
6	-0.298471	0.000000	-1.325127
6	1.104152	0.000000	-1.227317
7	-0.979967	0.000000	-0.030221
1	1.678266	0.000000	-2.151124
6	1.772528	0.000000	0.027851
1	2.847017	0.000000	0.176010
7	0.969135	0.000000	1.207999
8	-1.061708	0.000000	2.278695
1	-1.992753	0.000000	-0.058322
1	1.388962	0.000000	2.127929
6	-0.400204	0.000000	1.218312

----------uracil neutral----------
0 1

8	-0.993201	0.000000	-2.331437
6	-0.338697	0.000000	-1.296907
6	1.122400	0.000000	-1.199478
7	-0.990041	0.000000	-0.041622
1	1.698120	0.000000	-2.118425
6	1.715311	0.000000	0.020515
1	2.795602	0.000000	0.149405
7	0.980061	0.000000	1.186773
8	-1.050224	0.000000	2.263110
1	-2.007861	0.000000	-0.059339
1	1.428343	0.000000	2.096689
6	-0.415172	0.000000	1.219575

----------uracil cation----------
1 2

8	-0.963416	0.000000	-2.344782
6	-0.368262	0.000000	-1.282657
6	1.105311	0.000000	-1.198491
7	-1.034484	0.000000	-0.044950
1	1.673498	0.000000	-2.125759
6	1.742335	0.000000	0.061886
1	2.826716	0.000000	0.172371
7	1.002309	0.000000	1.161432
8	-1.008367	0.000000	2.271028
1	-2.057517	0.000000	-0.067217
1	1.428672	0.000000	2.094942
6	-0.458029	0.000000	1.202648

----------hypoxanthine
----------hypoxanthine anion----------
-1 2

1	-1.720771	0.000000	-3.106356
7	-1.688560	0.000000	-0.968058
6	-0.578466	0.000000	1.352183
6	0.630721	0.000000	-0.804567
8	-1.527538	0.000000	2.162584
6	-0.614838	0.000000	-0.094933
7	0.740928	0.000000	1.818362
7	0.238912	0.000000	-2.149596
1	0.819182	0.000000	2.829485
7	1.870471	0.000000	-0.341943
6	-1.164019	0.000000	-2.173549
1	0.872647	0.000000	-2.937506
6	1.932738	0.000000	1.028508
1	2.880182	0.000000	1.556499

----------hypoxanthine neutral----------
0 1

1	-1.681887	0.000000	-3.109536
7	-1.688168	0.000000	-0.975561
6	-0.594252	0.000000	1.348224
6	0.595518	0.000000	-0.799597
8	-1.503907	0.000000	2.163863
6	-0.619344	0.000000	-0.102020
7	0.770184	0.000000	1.793608
7	0.242597	0.000000	-2.127932
1	0.876325	0.000000	2.805830
7	1.866732	0.000000	-0.303512
6	-1.139370	0.000000	-2.170033

```
 1           0.887320    0.000000   -2.910949
 6           1.885452    0.000000    1.002298
 1           2.842059    0.000000    1.524295

---------------hypoxanthine cation---------------
 1  2
 1          -1.683027    0.000000   -3.100830
 7          -1.677891    0.000000   -0.947755
 6          -0.593444    0.000000    1.356943
 6           0.620607    0.000000   -0.823677
 8          -1.506756    0.000000    2.152732
 6          -0.640104    0.000000   -0.107346
 7           0.777544    0.000000    1.811845
 7           0.250093    0.000000   -2.147759
 1           0.890274    0.000000    2.829037
 7           1.840541    0.000000   -0.315716
 6          -1.117730    0.000000   -2.172974
 1           0.881407    0.000000   -2.948565
 6           1.863816    0.000000    1.025919
 1           2.834523    0.000000    1.521002

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