

Supporting Information: Revealing Non-Covalent Interactions

Erin R. Johnson, Shahar Keinan, Paula Mori-Sánchez,
Julia Contreras-García, Aron J. Cohen, and Weitao Yang

1 Gaussian Reference

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y. Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Wallingford, CT, 2004.

2 Molecular Geometries

The geometries of all species considered in this work (with the exception of the 2UXO pdb file, diamond, and graphite) are given in Å Cartesian coordinates. For diamond and graphite, the space group, lattice parameters (in Å), and internal coordinates of the atoms are given.

diamond

space group: 227 (Fd $\bar{3}$ m)

lattice parameter: a = 3.5667

C position: 0.125 0.125 0.125

graphite

space group: 186 (P6₃mc)

lattice parameter: a = 2.456

c = 6.696

C positions: 0 0 0
1/3 2/3 0

ethane

6	0.000000	0.000000	0.765057
6	0.000000	0.000000	-0.765057
1	0.000000	1.019538	1.164020
1	-0.882946	-0.509769	1.164020
1	0.882946	-0.509769	1.164020
1	0.000000	-1.019538	-1.164020
1	-0.882946	0.509769	-1.164020
1	0.882946	0.509769	-1.164020

n-octane

6	0.000000	0.766216	0.000000
6	0.000000	-0.766216	0.000000
6	-1.405575	1.376054	0.000000
6	1.405575	-1.376054	0.000000
6	-1.409950	2.908463	0.000000
6	1.409950	-2.908463	0.000000
6	-2.818879	3.507551	0.000000
6	2.818879	-3.507551	0.000000
1	0.553684	1.129401	0.877215
1	0.553684	1.129401	-0.877215
1	-0.553684	-1.129401	0.877215
1	-0.553684	-1.129401	-0.877215
1	-1.959575	1.012584	0.877049
1	-1.959575	1.012584	-0.877049
1	1.959575	-1.012584	0.877049
1	1.959575	-1.012584	-0.877049
1	-0.857070	3.271356	-0.876735
1	-0.857070	3.271356	0.876735
1	0.857070	-3.271356	-0.876735
1	0.857070	-3.271356	0.876735
1	-3.384207	3.189946	0.883382
1	-3.384207	3.189946	-0.883382
1	3.384207	-3.189946	0.883382
1	3.384207	-3.189946	-0.883382
1	-2.789442	4.601787	0.000000
1	2.789442	-4.601787	0.000000

branched octane

6	0.832643	1.172922	1.356619
---	----------	----------	----------

6	0.000000	0.000000	0.793403
1	1.898598	1.061219	1.140661
1	0.508191	2.140990	0.963394
1	0.724493	1.213629	2.445998
6	-1.432102	0.134629	1.356619
6	0.599459	-1.307551	1.356619
1	-2.108247	-0.630389	0.963394
1	-1.413279	0.020615	2.445998
1	-1.868342	1.113625	1.140661
1	0.688787	-1.234243	2.445998
1	-0.030256	-2.174844	1.140661
1	1.600056	-1.510601	0.963394
6	0.000000	0.000000	-0.793403
6	1.432102	0.134629	-1.356619
6	-0.599459	-1.307551	-1.356619
6	-0.832643	1.172922	-1.356619
1	1.868342	1.113625	-1.140661
1	2.108247	-0.630389	-0.963394
1	1.413279	0.020615	-2.445998
1	-1.600056	-1.510601	-0.963394
1	-0.688787	-1.234243	-2.445998
1	0.030256	-2.174844	-1.140661
1	-0.724493	1.213629	-2.445998
1	-1.898598	1.061219	-1.140661
1	-0.508191	2.140990	-0.963394

bicyclo[2,2,2]octene

6	-1.253462	0.777139	-0.671382
6	0.000000	1.288932	0.090123
6	0.000000	-1.288932	0.090123
6	-1.253462	-0.777139	-0.671382
1	-2.157689	1.166265	-0.194861
1	-1.238590	1.167834	-1.695145
1	-2.157689	-1.166265	-0.194861
1	-1.238590	-1.167834	-1.695145
6	0.000000	0.667552	1.466672
6	0.000000	-0.667552	1.466672
1	0.000000	-2.381295	0.131048
1	0.000000	2.381295	0.131048
6	1.253462	-0.777139	-0.671382
1	2.157689	-1.166265	-0.194861
1	1.238590	-1.167834	-1.695145
6	1.253462	0.777139	-0.671382
1	2.157689	1.166265	-0.194861
1	1.238590	1.167834	-1.695145
1	0.000000	-1.276429	2.364784
1	0.000000	1.276429	2.364784

methane dimer

6	-0.000000	0.000000	1.807279
1	-0.000000	1.026643	1.442400
1	-0.889099	-0.513322	1.442400
1	-0.000000	0.000000	2.896843
1	0.889099	-0.513322	1.442400
6	-0.000000	-0.000000	-1.807279
1	0.889099	0.513322	-1.442400
1	-0.000000	-0.000000	-2.896843
1	-0.889099	0.513322	-1.442400
1	-0.000000	-1.026643	-1.442400

benzene dimer

6	-1.800000	0.800000	1.391500
6	-1.800000	-0.405074	0.695750
6	-1.800000	-0.405074	-0.695750
6	-1.800000	0.800000	-1.391500
6	-1.800000	2.005074	-0.695750
6	-1.800000	2.005074	0.695750
6	1.800000	-0.800000	1.391500
6	1.800000	0.405074	0.695750
6	1.800000	0.405074	-0.695750
6	1.800000	-0.800000	-1.391500
6	1.800000	-2.005074	-0.695750
6	1.800000	-2.005074	0.695750
1	-1.800000	0.800000	2.471500
1	-1.800000	-1.340382	1.235750
1	-1.800000	-1.340382	-1.235750
1	-1.800000	0.800000	-2.471500
1	-1.800000	2.940382	-1.235750
1	-1.800000	2.940382	1.235750
1	1.800000	-0.800000	2.471500
1	1.800000	1.340382	1.235750
1	1.800000	1.340382	-1.235750
1	1.800000	-0.800000	-2.471500
1	1.800000	-2.940382	-1.235750
1	1.800000	-2.940382	1.235750

water dimer

8	1.531750	0.005922	-0.120880
1	0.575968	-0.005249	0.024966
1	1.906249	-0.037561	0.763218
8	-1.396226	-0.004990	0.106766
1	-1.789372	-0.742283	-0.371009
1	-1.777037	0.777638	-0.304264

formic acid dimer

6	-0.120234	1.914070	0.000000
1	-0.167295	3.007018	0.000000
8	-1.121857	1.220982	0.000000
8	1.121857	1.480489	0.000000
1	1.127582	0.489024	0.000000
8	1.121857	-1.220982	0.000000
6	0.120234	-1.914070	0.000000
8	-1.121857	-1.480489	0.000000
1	-1.127582	-0.489024	0.000000
1	0.167295	-3.007018	0.000000

alpha-helix

7	4.75399899	-0.11621726	1.47081515
6	5.58763100	-1.12174727	2.11768613
6	6.61609946	-1.70588026	1.12884677
8	7.70592166	-2.13447276	1.50443435
1	3.74460211	-0.26030045	1.41313530
1	6.14608228	-0.62701325	2.92117565
6	4.74288818	-2.25118656	2.68889053
1	4.04041352	-1.87252696	3.43839387
1	5.37338431	-3.00916044	3.16511341
1	4.15982493	-2.75069006	1.90650795
7	3.36104616	1.35954931	-0.43366101
6	4.28741673	2.07693909	0.42886926
6	5.28310669	1.09344559	1.07359250
8	6.45471991	1.39794827	1.29262119
1	2.35876192	1.38962321	-0.23736308
1	4.86187670	2.76970584	-0.19738307
6	3.55118976	2.84379885	1.51768281
1	2.87500996	3.58563198	1.08053011
1	4.25703588	3.36843520	2.17052503
1	2.95345475	2.17603604	2.14537596
7	1.80093319	-0.66577164	-1.53283369
6	2.72157213	0.03035328	-2.41979819
6	3.80124912	0.75344923	-1.59159842
8	4.96580076	0.84858004	-1.97656025
1	0.80919366	-0.42183271	-1.54061310
1	3.22426251	-0.72115138	-3.03978780
6	1.99303274	1.03334085	-3.30083807
1	1.25406025	0.53126984	-3.93371908
1	2.69723643	1.56366063	-3.95165763
1	1.46597091	1.78472827	-2.70327654
7	0.30785470	-1.36188346	0.70900239
6	1.15161521	-2.39126334	0.11635386
6	2.22313490	-1.74262814	-0.78089300
8	3.36071811	-2.20299127	-0.87932178

1	-0.69398049	-1.35525171	0.51288184
1	1.66890041	-2.91137849	0.93100179
6	0.33108052	-3.37832951	-0.69876957
1	-0.40422856	-3.88828279	-0.06753728
1	0.97548671	-4.13871429	-1.15324250
1	-0.21253182	-2.87899280	-1.50801951
7	-1.04523335	1.03769793	1.11908514
6	-0.17847254	0.56023907	2.18809156
6	0.81793620	-0.47722854	1.63578043
8	1.97396232	-0.55911162	2.05287246
1	-2.05434084	0.89505091	1.18690769
1	0.39998086	1.41512253	2.55807526
6	-0.98299554	-0.05675620	3.32147966
1	-1.66328927	0.67994164	3.76205966
1	-0.32262383	-0.42654942	4.11232489
1	-1.58704834	-0.90077261	2.97332663
7	-2.50884081	1.16431957	-1.24801924
6	-1.56667219	2.24291120	-0.97735268
6	-0.54085701	1.79706118	0.08447122
8	0.63476661	2.16046284	0.05200075
1	-3.50444813	1.31339380	-1.08924918
1	-1.01880778	2.44988220	-1.90358029
6	-2.28232564	3.49785016	-0.50003273
1	-2.97635513	3.86265641	-1.26359639
1	-1.56515651	4.29584095	-0.28124482
1	-2.85707112	3.31012562	0.41308070
7	-4.07314639	-1.12993176	-0.95025102
6	-3.17694820	-1.06287050	-2.09664869
6	-2.08657790	-0.00111160	-1.85562868
8	-0.92878242	-0.15275263	-2.24751977
1	-5.07212531	-0.97148352	-1.08566246
1	-2.68099555	-2.03624866	-2.19340054
6	-3.93498934	-0.73206172	-3.37367382
1	-4.67926036	-1.50400522	-3.59529486
1	-3.25104140	-0.66276370	-4.22652961
1	-4.46100620	0.22528131	-3.29205531
7	-5.50622918	-0.41853668	1.32572959
6	-4.67263824	-1.61090988	1.40268599
6	-3.62390175	-1.58822464	0.27218912
8	-2.48061776	-2.01463395	0.43174413
1	-6.51600188	-0.50849094	1.21725684
1	-4.13829184	-1.58602987	2.35966870
6	-5.51366911	-2.87443692	1.30282355
1	-6.25511338	-2.91390695	2.10845157
1	-4.88386215	-3.76761471	1.37065884
1	-6.05492900	-2.92368710	0.35169730
7	-6.85348267	1.73910927	0.29575047

6	-5.94748042	2.00750642	1.40640923
6	-4.96663590	0.83204510	1.55101452
8	-3.79920538	0.98998831	1.90483500
1	-7.71547745	1.23289492	0.47300176
1	-5.36301996	2.90212610	1.16372096
6	-6.71277882	2.22386787	2.70273292
1	-7.41672359	3.05632740	2.60479985
1	-6.02621409	2.44903294	3.52505133
1	-7.28543472	1.33535348	2.98851850
7	-8.38757343	0.49349895	-1.61626979
6	-7.48498871	1.53923779	-2.08398240
6	-6.42361251	1.86135178	-1.01135566
8	-5.30540828	2.28596251	-1.29778373
1	-9.35692515	0.70117883	-1.40563431
1	-6.95953753	1.16305634	-2.96965309
6	-8.26009950	2.80261222	-2.42549862
1	-8.99964346	2.60603233	-3.20814226
1	-7.58736127	3.59106208	-2.77969925
1	-8.79589017	3.19128524	-1.55162011
7	-9.99105849	-1.17282545	-0.11678332
6	-9.03361680	-1.80795522	-1.01680531
6	-7.95574964	-0.80984534	-1.47784332
8	-6.81292906	-1.15700039	-1.76834891
1	-10.99431129	-1.24212649	-0.27846260
1	-8.53246850	-2.60300676	-0.45347109
6	-9.74158103	-2.38222125	-2.23485669
1	-10.48675767	-3.12755109	-1.93699732
1	-9.02745982	-2.86273728	-2.91225853
1	-10.26139363	-1.60095627	-2.80075499
7	6.18427798	-1.82287757	-0.17546295
6	7.04986194	-2.35631108	-1.22040223
6	8.12281159	-1.33418749	-1.65152102
8	9.19335270	-1.68454622	-2.14552456
1	5.21105693	-1.60702338	-0.39128638
1	7.57545950	-3.22740974	-0.81147031
6	6.23597197	-2.76767670	-2.43954761
1	5.50287017	-3.53772479	-2.17701820
1	6.88417130	-3.16877653	-3.22595116
1	5.69070826	-1.91667888	-2.86245090
7	7.74267755	-0.01080574	-1.58168642
6	8.64589637	1.06667228	-1.97155802
6	9.70860273	1.34676954	-0.88744976
8	10.77354696	1.90812057	-1.14311324
1	6.77803209	0.20987513	-1.33325113
1	9.17956582	0.75382972	-2.87696813
6	7.87254633	2.34919657	-2.24633458
1	7.15011043	2.20234856	-3.05625559

1	8.54763095	3.16134881	-2.53601629
1	7.31907395	2.67925555	-1.35993602
7	9.32119364	1.05603404	0.40110449
6	10.19109756	1.24653222	1.55103998
6	11.12571496	0.05507748	1.83303982
8	11.85579573	0.04319741	2.83157671
1	8.38728851	0.67358898	0.54473935
1	10.84421040	2.10119321	1.33820388
6	9.36055795	1.54935055	2.79305167
1	8.72110951	2.42386319	2.63172492
1	9.99920299	1.75464208	3.65880677
1	8.71350363	0.70340735	3.05102417
6	11.18413201	-1.07964491	0.84344720
1	11.58949622	-0.72553395	-0.10691604
1	10.19141101	-1.50951876	0.70457860
1	11.84224324	-1.86355691	1.22964997
7	-11.92988823	0.18561003	1.27231469
6	-10.79036957	-0.35515719	2.05426675
6	-9.61316600	-0.68461739	1.11608940
8	-8.43331597	-0.53517343	1.43144538
1	-12.77507645	0.12513301	1.84586103
1	-10.45414338	0.36955732	2.80590085
6	-11.22211935	-1.63991330	2.75731360
1	-12.02918156	-1.44533609	3.47246413
1	-10.38289552	-2.07829628	3.30926897
1	-11.57232712	-2.39644279	2.04529418
6	-11.72226766	1.59264106	0.93644211
1	-11.63803871	2.21010077	1.83628820
1	-10.82818862	1.73333512	0.32138776
1	-12.57781515	1.95539433	0.35888038

beta-sheet

7	-1.45231726	-2.55315573	-0.08425553
6	-0.19683941	-1.83154848	-0.11998158
6	0.98965185	-2.78990905	-0.07336086
8	0.85321402	-4.00984086	-0.00910281
1	-1.39696059	-3.56719429	-0.02168213
1	-0.15696307	-1.24788285	-1.04428743
1	-0.15761625	-1.16088417	0.74431867
7	2.21114492	-2.16553422	-0.11003184
6	3.44883595	-2.91265279	-0.07460941
6	4.65935334	-1.98372621	-0.17297132
8	4.56646538	-0.75458854	-0.18380715
1	2.25608266	-1.14158710	-0.15240992
1	3.49529421	-3.47099038	0.86475727
1	3.45841066	-3.61854913	-0.91212400
7	5.86726192	-2.63646170	-0.23802694

6	7.10797152	-1.89794674	-0.32675325
6	8.32448631	-2.81651193	-0.43331189
8	8.24721242	-4.04091951	-0.37274106
1	5.92839834	-3.65114846	-0.22349700
1	7.06293168	-1.25728631	-1.21283825
1	7.20324829	-1.27803028	0.56968186
7	9.50638998	-2.13745881	-0.59175300
6	10.77778918	-2.80396639	-0.74847799
6	11.90596373	-1.77028353	-0.70217553
8	11.84063497	-0.67801757	-1.26461595
1	9.48147393	-1.11094031	-0.64371415
1	10.88916216	-3.55222855	0.04136365
1	10.79458516	-3.30600062	-1.72083725
7	12.99371274	-2.12707870	0.06627830
6	14.20487437	-1.31442449	0.06162510
6	14.10894685	0.03028950	0.79955951
8	15.01593993	0.85580370	0.75331165
1	13.03125163	-3.04317763	0.49673804
1	14.99320594	-1.90551990	0.53716325
1	14.48146302	-1.11267099	-0.97843656
7	12.97105039	0.20526397	1.55091734
6	12.66929208	1.44268231	2.25046775
6	11.56649943	2.26941752	1.57710362
8	10.99414175	3.18317625	2.16814395
1	12.26705080	-0.52075799	1.53413394
1	12.32403965	1.16725585	3.25129192
1	13.56317876	2.06723646	2.33359253
7	11.30958847	1.96669420	0.26121899
6	10.24268587	2.60818189	-0.47844943
6	8.98205897	1.74480453	-0.39230790
8	9.02227727	0.51323188	-0.36906328
1	11.77498323	1.17041133	-0.17038999
1	10.05103303	3.61171958	-0.08805696
1	10.54642521	2.67716153	-1.52675388
7	7.79471683	2.43258543	-0.39127446
6	6.52728454	1.73213089	-0.33275248
6	5.33862202	2.68704497	-0.35090555
8	5.46568369	3.90792935	-0.41407727
1	7.76650534	3.44915460	-0.37826522
1	6.46352696	1.06451720	-1.19792237
1	6.50157781	1.14005286	0.58775160
7	4.12230125	2.05283609	-0.29686969
6	2.87817520	2.79089744	-0.30440741
6	1.67037533	1.85247946	-0.28381136
8	1.76701045	0.62671797	-0.21965987
1	4.08544948	1.02863787	-0.24431546
1	2.85194347	3.43794062	0.57810549

1	2.84369655	3.41286323	-1.20445562
7	0.46049460	2.49974711	-0.33868577
6	-0.79293770	1.77318728	-0.32514728
6	-1.98235939	2.72674979	-0.40021780
8	-1.84916943	3.94708698	-0.47721503
1	0.40228479	3.51362923	-0.39260845
1	-0.81288347	1.09800117	-1.18571447
1	-0.84814049	1.19440371	0.60251496
7	-3.20093110	2.09932700	-0.37616331
6	-4.44178740	2.83935897	-0.44373789
6	-5.65107670	1.90858138	-0.34512001
8	-5.55470673	0.68300655	-0.27053325
1	-3.24228307	1.07550644	-0.31491392
1	-4.46638488	3.56191876	0.37929754
1	-4.47539953	3.38026087	-1.39501984
7	-6.86063920	2.55842524	-0.35163884
6	-8.11241452	1.83258006	-0.26274955
6	-9.30414607	2.78468457	-0.27086830
8	-9.17846253	4.00205972	-0.38796392
1	-6.92170974	3.57040489	-0.42122028
1	-8.18227681	1.15469504	-1.11821209
1	-8.11178387	1.25721809	0.66789926
7	-5.11241031	-2.08732934	-0.08736409
6	-3.87318593	-2.83279448	-0.08250169
6	-2.66018126	-1.90226548	-0.13042308
8	-2.75193210	-0.67701254	-0.20996564
1	-5.07037120	-1.06455552	-0.15557280
1	-3.83187602	-3.44016489	0.82780852
1	-3.85937279	-3.49469014	-0.95423579
7	-8.77426549	-2.46971670	0.07012410
6	-7.51919451	-1.75321668	-0.03183450
6	-6.33146989	-2.71118495	-0.01173405
8	-6.46425680	-3.93201762	0.06365320
1	-8.72112407	-3.48211864	0.14344060
1	-7.51632340	-1.19071307	-0.97069308
1	-7.44353056	-1.06414449	0.81418411
7	-12.41490859	-2.02526371	0.45983214
6	-11.19093086	-2.74371187	0.18237447
6	-9.98207947	-1.81388659	0.07897106
8	-10.07287799	-0.58986706	-0.01796610
1	-12.42342999	-1.00262792	0.38708301
1	-11.02231991	-3.47874418	0.97688365
1	-11.31160039	-3.27452992	-0.76833477
7	-10.51762124	2.15834545	-0.13841708
6	-11.75776151	2.89821485	-0.13246982
6	-12.95819589	1.99854033	0.16811139
8	-12.87811752	0.77509162	0.26591589

1	-10.55540637	1.13501605	-0.06338232
1	-11.69333229	3.68937816	0.62279536
1	-11.89017350	3.35814799	-1.11710812
6	-14.75065954	-1.79736156	1.00434395
6	-13.57267325	-2.69566658	0.75643793
8	-13.65151314	-3.91875508	0.81062068
1	-15.01313286	-1.27367388	0.08119068
1	-14.50836758	-1.07011446	1.78405431
7	-14.14413103	2.69071462	0.30354989
6	-15.38258092	2.01076729	0.58227285
1	-14.15002647	3.69858742	0.21301992
1	-15.58982377	1.29610917	-0.21986690
1	-15.29601355	1.47784907	1.53255347
1	-15.60688071	-2.39241861	1.33275438
1	-16.18445681	2.74979261	0.63981095

DNA helix

15	-5.73800	7.65000	1.88000
8	-6.55000	8.71700	1.25100
8	-4.90600	8.06100	3.03200
8	-6.68700	6.43500	2.30700
6	-6.99800	5.41800	1.33600
6	-6.89800	4.04500	1.97200
8	-5.55100	3.49600	1.89500
6	-7.24000	3.97500	3.46000
8	-7.91500	2.75000	3.71900
6	-5.88400	3.94200	4.16800
6	-5.19200	3.01100	3.18000
7	-3.72500	3.02800	3.28000
6	-3.06000	1.82300	3.25600
8	-3.63100	0.75000	3.15400
7	-1.69400	1.92300	3.35400
6	-0.94700	3.07900	3.47200
8	0.27700	3.01200	3.55100
6	-1.71000	4.30600	3.49100
6	-0.98700	5.61000	3.61700
6	-3.04300	4.21900	3.39600
15	-9.23500	3.06300	5.27700
8	-10.52500	3.44600	4.65900
8	-8.79300	3.88800	6.42300
8	-9.28500	1.52400	5.71100
6	-8.94800	0.51400	4.74100
6	-8.05500	-0.53500	5.37200
8	-6.64300	-0.18900	5.28000
6	-8.27600	-0.78700	6.86400
8	-8.09900	-2.17400	7.12800
6	-7.15300	-0.01400	7.55800

6	-6.05500	-0.36500	6.56100
7	-4.88600	0.50400	6.64600
6	-4.87800	1.87500	6.75900
7	-3.67500	2.37700	6.81400
6	-2.83600	1.27300	6.73200
6	-1.42000	1.19000	6.74100
8	-0.59600	2.10900	6.82600
7	-0.98200	-0.12500	6.63700
6	-1.80200	-1.22300	6.53700
7	-1.18800	-2.41200	6.44500
7	-3.12300	-1.16000	6.52900
6	-3.57000	0.10900	6.62800
15	-9.25100	-2.69800	8.69800
8	-10.52500	-3.14800	8.09400
8	-9.36600	-1.76500	9.84000
8	-8.38200	-3.97000	9.12900
6	-7.52600	-4.59400	8.15300
6	-6.18000	-4.91500	8.77300
8	-5.24200	-3.80500	8.66700
6	-6.19700	-5.24300	10.26500
8	-5.23600	-6.26000	10.52400
6	-5.73500	-3.95400	10.94900
6	-4.65100	-3.59700	9.94000
7	-4.21200	-2.19600	10.01600
6	-2.86100	-1.93600	9.96700
8	-2.01900	-2.81300	9.86500
7	-2.53200	-0.60500	10.04300
6	-3.39900	0.46400	10.16000
8	-2.95500	1.60800	10.21800
6	-4.80100	0.11800	10.20500
6	-5.81500	1.21100	10.33200
6	-5.13200	-1.17700	10.13200
15	-5.91800	-7.39800	12.10600
8	-6.69100	-8.51400	11.51400
8	-6.54900	-6.70700	13.25300
8	-4.46400	-7.91600	12.52500
6	-3.41400	-7.92100	11.53900
6	-2.13100	-7.38700	12.14400
8	-2.02500	-5.93900	12.03200
6	-1.93700	-7.65600	13.63700
8	-0.56000	-7.91400	13.88300
6	-2.31400	-6.34000	14.32000
6	-1.65600	-5.41800	13.30000
7	-2.12000	-4.03600	13.37400
6	-3.41900	-3.60300	13.50200
7	-3.52300	-2.30300	13.54100
6	-2.21600	-1.84800	13.43400

6	-1.70000	-0.52700	13.41700
8	-2.31700	0.54200	13.49800
7	-0.31500	-0.51900	13.29200
6	0.47400	-1.64000	13.19500
7	1.79400	-1.42500	13.08000
7	0.00600	-2.87600	13.21000
6	-1.33800	-2.90700	13.33000
15	-0.39400	-9.15000	15.46700
8	-0.36900	-10.50900	14.88100
8	-1.29900	-8.95700	16.62100
8	1.09100	-8.71300	15.87000
6	1.93400	-8.10400	14.87300
6	2.66500	-6.91600	15.46700
8	1.89800	-5.68200	15.35600
6	2.99400	-7.01300	16.95600
8	4.26200	-6.41200	17.18700
6	1.92200	-6.16700	17.64500
6	1.90300	-5.03800	16.62100
7	0.70700	-4.18700	16.70400
6	0.87700	-2.82300	16.63500
8	1.96900	-2.29400	16.50900
7	-0.28600	-2.09700	16.71900
6	-1.56900	-2.58800	16.86200
8	-2.51900	-1.81200	16.92400
6	-1.67300	-4.02900	16.92800
6	-3.02300	-4.65300	17.08300
6	-0.54500	-4.74500	16.84600
15	5.15800	-7.39200	18.76900
8	5.97100	-8.47900	18.17900
8	4.32300	-7.76200	19.93400
8	6.10600	-6.16300	19.15800
6	6.42000	-5.17900	18.15400
6	6.31900	-3.78600	18.74300
8	4.97300	-3.23900	18.64400
6	6.65700	-3.66600	20.22900
8	7.33200	-2.43300	20.44900
6	5.29900	-3.60800	20.93200
6	4.61100	-2.71000	19.91100
7	3.15400	-2.72300	20.00700
6	2.34300	-3.82300	20.16100
7	1.07500	-3.51900	20.21600
6	1.04500	-2.13600	20.09100
6	-0.05100	-1.23700	20.07900
8	-1.25800	-1.49300	20.18200
7	0.36700	0.08100	19.93100
6	1.67500	0.48200	19.80800
7	1.87700	1.80200	19.67300

7	2.70600	-0.34500	19.81800
6	2.32200	-1.63100	19.96100
15	-5.90600	7.84200	21.19400
8	-6.68400	8.94800	21.79600
8	-6.53400	7.15800	20.04200
8	-4.45400	8.37000	20.77900
6	-3.40300	8.37200	21.76500
6	-2.11900	7.84900	21.15500
8	-2.00600	6.40000	21.25500
6	-1.92700	8.13200	19.66400
8	-0.55000	8.39900	19.42000
6	-2.29800	6.82100	18.97000
6	-1.63500	5.89300	19.98200
7	-2.09600	4.50000	19.89500
6	-1.13800	3.48500	19.94900
8	0.05700	3.79400	20.06600
7	-1.53600	2.19400	19.87100
6	-2.83300	1.90400	19.74500
7	-3.18100	0.61600	19.67100
6	-3.83100	2.91900	19.68800
6	-3.42200	4.19100	19.76600
15	-0.39900	9.59400	17.85300
8	-0.37800	10.94600	18.45200
8	-1.29900	9.41100	16.69100
8	1.08700	9.15900	17.45300
6	1.92500	8.54100	18.44900
6	2.65800	7.35800	17.84800
8	1.89100	6.12400	17.94200
6	2.99600	7.46900	16.36100
8	4.26500	6.86900	16.13100
6	1.92800	6.63100	15.65800
6	1.90200	5.49200	16.67100
7	0.71600	4.64700	16.57400
6	-0.59000	5.05000	16.42900
7	-1.44500	4.05800	16.37000
6	-0.64900	2.92500	16.48500
6	-0.95400	1.55300	16.49400
7	-2.19200	1.06800	16.38200
7	0.07300	0.68500	16.62400
6	1.31300	1.17200	16.73700
7	1.72700	2.43800	16.74200
6	0.68400	3.27400	16.61100
15	5.10400	7.86000	14.56200
8	5.90500	8.94800	15.16600
8	4.27900	8.23400	13.39100
8	6.06200	6.63900	14.17600
6	6.37200	5.65000	15.17700

6	6.28300	4.26100	14.58000
8	4.93800	3.70600	14.66200
6	6.63600	4.15000	13.09600
8	7.32000	2.92100	12.87600
6	5.28700	4.09000	12.38000
6	4.59200	3.18300	13.38900
7	3.12700	3.19000	13.27700
6	2.45700	1.96500	13.33200
8	3.11800	0.92600	13.47100
7	1.10700	1.94400	13.23200
6	0.43300	3.08600	13.08200
7	-0.89800	3.01800	12.98600
6	1.09000	4.34800	13.02300
6	2.42600	4.35400	13.12400
15	8.53000	3.13100	11.32700
8	9.81200	3.53600	11.94400
8	8.09800	3.91800	10.15000
8	8.58300	1.57900	10.94500
6	8.23700	0.60200	11.94500
6	7.34900	-0.46800	11.33900
8	5.93700	-0.12000	11.40600
6	7.58500	-0.77000	9.86000
8	7.41100	-2.16500	9.64100
6	6.47000	-0.02100	9.13000
6	5.36100	-0.33800	10.12700
7	4.19300	0.52800	10.00100
6	4.17400	1.89200	9.84100
7	2.96800	2.39700	9.75700
6	2.13500	1.29200	9.86900
6	0.73600	1.15700	9.85600
7	-0.10600	2.18300	9.71800
7	0.22600	-0.08700	9.99000
6	1.07100	-1.11400	10.12800
7	2.40100	-1.11600	10.15600
6	2.87700	0.13300	10.02000
15	8.63900	-2.67200	8.09800
8	9.91100	-3.09100	8.72800
8	8.75900	-1.78500	6.92000
8	7.78000	-3.96500	7.71000
6	6.91900	-4.55500	8.70300
6	5.58100	-4.90700	8.08600
8	4.63600	-3.79900	8.14200
6	5.61100	-5.29200	6.60700
8	4.65600	-6.32500	6.38200
6	5.14800	-4.03500	5.87000
6	4.05400	-3.64400	6.85600
7	3.60900	-2.25000	6.72300

6	2.23700	-1.99100	6.75100
8	1.45000	-2.94100	6.88700
7	1.80100	-0.71600	6.63000
6	2.68100	0.27700	6.48500
7	2.20600	1.52100	6.36800
6	4.08500	0.04200	6.45300
6	4.50100	-1.22500	6.57400
15	5.25700	-7.42600	4.85400
8	6.02800	-8.51400	5.49600
8	5.89200	-6.78400	3.68100
8	3.80400	-7.96100	4.45200
6	2.75100	-7.92400	5.43400
6	1.47000	-7.41700	4.80100
8	1.36300	-5.96600	4.85100
6	1.28100	-7.75000	3.32200
8	-0.09600	-8.01800	3.08200
6	1.66100	-6.46500	2.58500
6	0.99900	-5.49900	3.56000
7	1.46300	-4.12200	3.42900
6	2.75800	-3.68300	3.28600
7	2.86600	-2.38100	3.19000
6	1.55600	-1.93000	3.27500
6	0.99500	-0.64200	3.23900
7	1.71300	0.47500	3.10200
7	-0.34800	-0.53900	3.34900
6	-1.06600	-1.65900	3.48700
7	-0.65600	-2.92500	3.53500
6	0.68100	-2.99200	3.42200
1	-8.05800	5.57800	0.94818
1	-6.25602	5.48539	0.47314
1	-7.66642	3.46091	1.36540
1	-7.89792	4.84154	3.80037
1	-5.39212	4.96912	4.21964
1	-5.88337	3.62215	5.26221
1	-5.51532	1.93818	3.39002
1	-1.14105	0.99254	3.33689
1	-1.74398	6.45845	3.69898
1	-0.33287	5.59301	4.55050
1	-0.33318	5.77204	2.69729
1	-3.62704	5.15279	3.41151
1	-9.90335	0.01905	4.36425
1	-8.39513	1.00109	3.87113
1	-8.34005	-1.46111	4.77144
1	-9.31459	-0.47154	7.21244
1	-7.35810	1.10634	7.60672
1	-6.95428	-0.26775	8.65149
1	-5.68412	-1.42217	6.77182

1	-5.79343	2.48630	6.79895
1	0.08670	-0.29727	6.63460
1	-0.10682	-2.46484	6.45234
1	-1.77367	-3.31872	6.36341
1	-8.01194	-5.55768	7.78587
1	-7.37387	-3.87969	7.27766
1	-5.87104	-5.83407	8.17346
1	-7.21925	-5.59689	10.62467
1	-6.55873	-3.16776	11.00281
1	-5.41378	-4.03810	12.03957
1	-3.72764	-4.23373	10.14389
1	-1.47655	-0.36717	10.00728
1	-6.86312	0.76561	10.28025
1	-5.67716	1.74285	11.33087
1	-5.67723	1.95744	9.48144
1	-6.20034	-1.44298	10.16663
1	-3.24388	-8.98762	11.17432
1	-3.71950	-7.25691	10.66421
1	-1.34753	-7.95164	11.53823
1	-2.55302	-8.54119	14.00653
1	-3.44193	-6.18760	14.38434
1	-1.99446	-6.21514	15.40715
1	-0.53278	-5.39009	13.49284
1	-4.28274	-4.28364	13.56510
1	0.17936	0.44376	13.26938
1	2.17855	-0.41318	13.06797
1	2.47394	-2.26344	12.99929
1	2.69436	-8.86874	14.50336
1	1.28817	-7.74908	14.00321
1	3.62582	-6.91572	14.85346
1	3.01940	-8.08941	17.33055
1	0.92046	-6.70629	17.72045
1	2.11724	-5.87388	18.72923
1	2.79694	-4.35411	16.80203
1	-0.18586	-1.02038	16.66739
1	-2.92105	-5.78837	17.07129
1	-3.48262	-4.32306	18.07269
1	-3.69472	-4.32322	16.22298
1	-0.62190	-5.84273	16.89481
1	7.48093	-5.35228	17.77452
1	5.68018	-5.27505	17.29200
1	7.08946	-3.22330	18.11901
1	7.31346	-4.52113	20.59969
1	4.80584	-4.63231	21.01680
1	5.29557	-3.25170	22.01488
1	4.93489	-1.63092	20.08503
1	2.72426	-4.85406	20.23072

1	-0.39584	0.84878	19.91123
1	1.03369	2.48067	19.66588
1	2.88323	2.18795	19.57123
1	-3.23747	9.43643	22.13809
1	-3.70484	7.69980	22.63485
1	-1.33762	8.41185	21.76511
1	-2.54738	9.01731	19.30212
1	-3.42524	6.66389	18.90480
1	-1.97844	6.70711	17.88165
1	-0.51170	5.87290	19.78862
1	-2.42072	-0.15339	19.71366
1	-4.22320	0.34196	19.56839
1	-4.89813	2.66668	19.58375
1	-4.16575	5.00248	19.72562
1	2.68397	9.30209	18.82887
1	1.27502	8.17907	19.31279
1	3.61464	7.35139	18.46800
1	3.02452	8.54907	15.99737
1	0.92736	7.17185	15.58186
1	2.12945	6.34816	14.57217
1	2.79632	4.80916	16.48792
1	-0.89031	6.10802	16.36804
1	-3.03075	1.74419	16.27676
1	-2.35761	-0.00166	16.39637
1	2.10775	0.41647	16.84109
1	7.42874	5.82609	15.56673
1	5.62390	5.73741	16.03275
1	7.04990	3.69949	15.20943
1	7.29194	5.01012	12.73609
1	4.79028	5.11264	12.29592
1	5.29627	3.73958	11.29523
1	4.92259	2.10639	13.21229
1	-1.39552	2.05764	13.03069
1	-1.47878	3.92327	12.86354
1	0.52165	5.28338	12.89908
1	2.96831	5.31188	13.08313
1	9.18859	0.11985	12.34699
1	7.67657	1.11718	12.79359
1	7.62794	-1.37370	11.97263
1	8.62712	-0.46663	9.51136
1	6.67626	1.09703	9.04592
1	6.28220	-0.31150	8.04375
1	4.99038	-1.40112	9.94807
1	5.08796	2.50453	9.78820
1	0.27951	3.18850	9.60774
1	-1.17455	2.00980	9.71631
1	0.59672	-2.10250	10.23395

1	7.40680	-5.50092	9.11152
1	6.75605	-3.80772	9.54835
1	5.27283	-5.80428	8.71808
1	6.63789	-5.65294	6.26815
1	5.96803	-3.24699	5.79131
1	4.83557	-4.16408	4.78127
1	3.13563	-4.29301	6.66896
1	1.13821	1.69718	6.39244
1	2.88913	2.35223	6.24882
1	4.80113	0.87034	6.33335
1	5.58011	-1.44498	6.55312
1	2.57986	-8.97390	5.84391
1	3.05315	-7.22313	6.28081
1	0.68443	-7.95593	5.42713
1	1.89748	-8.65080	2.99319
1	2.78926	-6.31564	2.51934
1	1.34593	-6.38767	1.49214
1	-0.12321	-5.47795	3.36050
1	3.62414	-4.36281	3.25503
1	2.79019	0.41829	3.01116
1	1.21805	1.43751	3.08175
1	-2.15434	-1.51294	3.57349

A-T base pair

7	-4.21200000	-2.19600000	10.01600000
6	-2.86100000	-1.93600000	9.96700000
8	-2.01900000	-2.81300000	9.86500000
7	-2.53200000	-0.60500000	10.04300000
6	-3.39900000	0.46400000	10.16000000
8	-2.95500000	1.60800000	10.21800000
6	-4.80100000	0.11800000	10.20500000
6	-5.13200000	-1.17700000	10.13200000
7	4.19300000	0.52800000	10.00100000
6	4.17400000	1.89200000	9.84100000
7	2.96800000	2.39700000	9.75700000
6	2.13500000	1.29200000	9.86900000
6	0.73600000	1.15700000	9.85600000
7	-0.10600000	2.18300000	9.71800000
7	0.22600000	-0.08700000	9.99000000
6	1.07100000	-1.11400000	10.12800000
7	2.40100000	-1.11600000	10.15600000
6	2.87700000	0.13300000	10.02000000
1	-1.47655000	-0.36717000	10.00728000
1	-6.20034000	-1.44298000	10.16663000
1	5.08796000	2.50453000	9.78820000
1	0.27951000	3.18850000	9.60774000
1	-1.17455000	2.00980000	9.71631000

1	0.59672000	-2.10250000	10.23395000
1	-4.51061196	-3.14897347	9.96430408
1	-5.52609884	0.89959076	10.29581613
1	4.99328989	-0.06536562	10.08733264

C-G base pair

7	-2.12000000	-4.03600000	13.37400000
6	-3.41900000	-3.60300000	13.50200000
7	-3.52300000	-2.30300000	13.54100000
6	-2.21600000	-1.84800000	13.43400000
6	-1.70000000	-0.52700000	13.41700000
8	-2.31700000	0.54200000	13.49800000
7	-0.31500000	-0.51900000	13.29200000
6	0.47400000	-1.64000000	13.19500000
7	1.79400000	-1.42500000	13.08000000
7	0.00600000	-2.87600000	13.21000000
6	-1.33800000	-2.90700000	13.33000000
7	3.12700000	3.19000000	13.27700000
6	2.45700000	1.96500000	13.33200000
8	3.11800000	0.92600000	13.47100000
7	1.10700000	1.94400000	13.23200000
6	0.43300000	3.08600000	13.08200000
7	-0.89800000	3.01800000	12.98600000
6	1.09000000	4.34800000	13.02300000
6	2.42600000	4.35400000	13.12400000
1	-4.28274000	-4.28364000	13.56510000
1	0.17936000	0.44376000	13.26938000
1	2.17855000	-0.41318000	13.06797000
1	2.47394000	-2.26344000	12.99929000
1	-1.39552000	2.05764000	13.03069000
1	-1.47878000	3.92327000	12.86354000
1	0.52165000	5.28338000	12.89908000
1	2.96831000	5.31188000	13.08313000
1	4.12407909	3.18523580	13.35322721
1	-1.80212437	-4.98277613	13.32330432