

Supplementary Information for:

Theoretical Characterization of the Conformational Feature for Unnatural Oligonucleotide Containing a Six Nucleotide Genetic Alphabet

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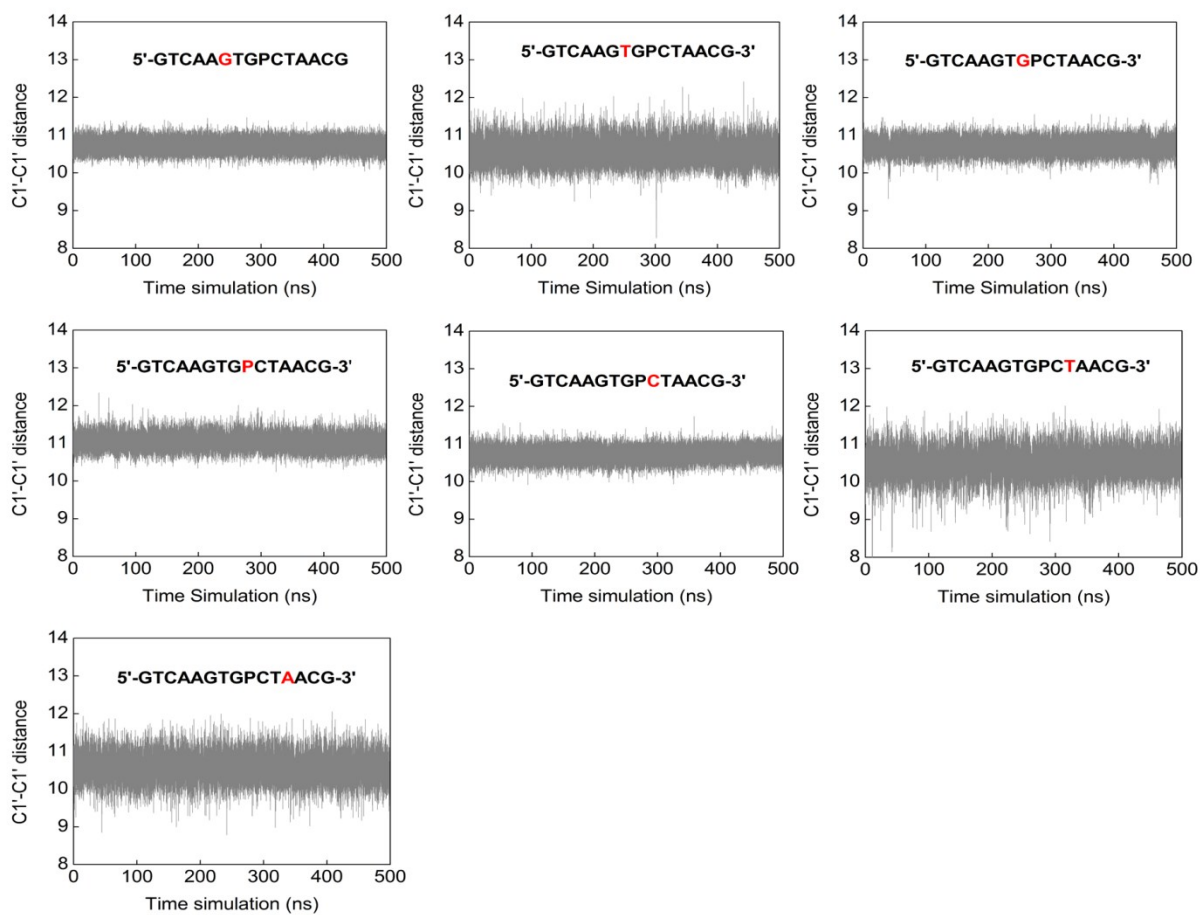


Fig. S1 Time evolution of the C1'-C1' distances for natural and unnatural residues of the sequence 5'-GTCAAGTGPCTAACG-3'. (The highlighted letter in each of the Figure shows the respective position of the residue in the sequence.)

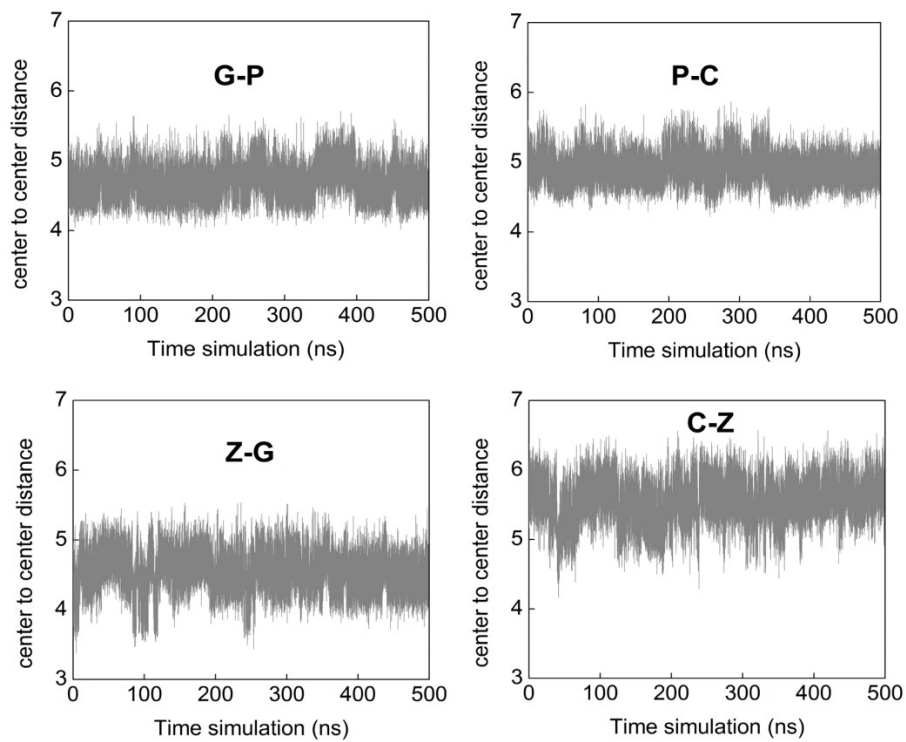


Fig. S2 Time evolution of the center-to-center distances between unnatural base and their neighboring stacked natural bases. (a) G-P, (b) P-C, (c) C-Z, and (d) Z-G.

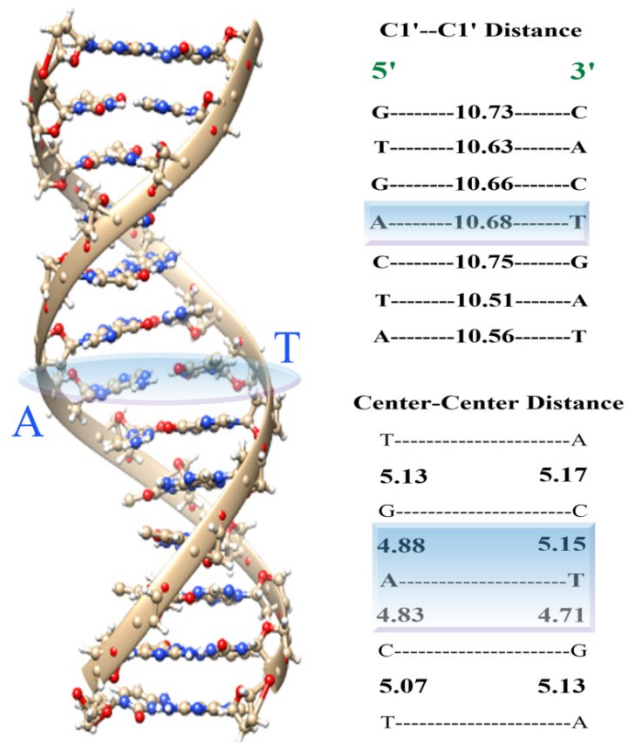


Fig. S3 MD average conformation of natural oligonucleotides containing AT^{9th} of the production run, along with the average C1'-C1' distances and the center-to-center distance of neighboring stacked natural bases.

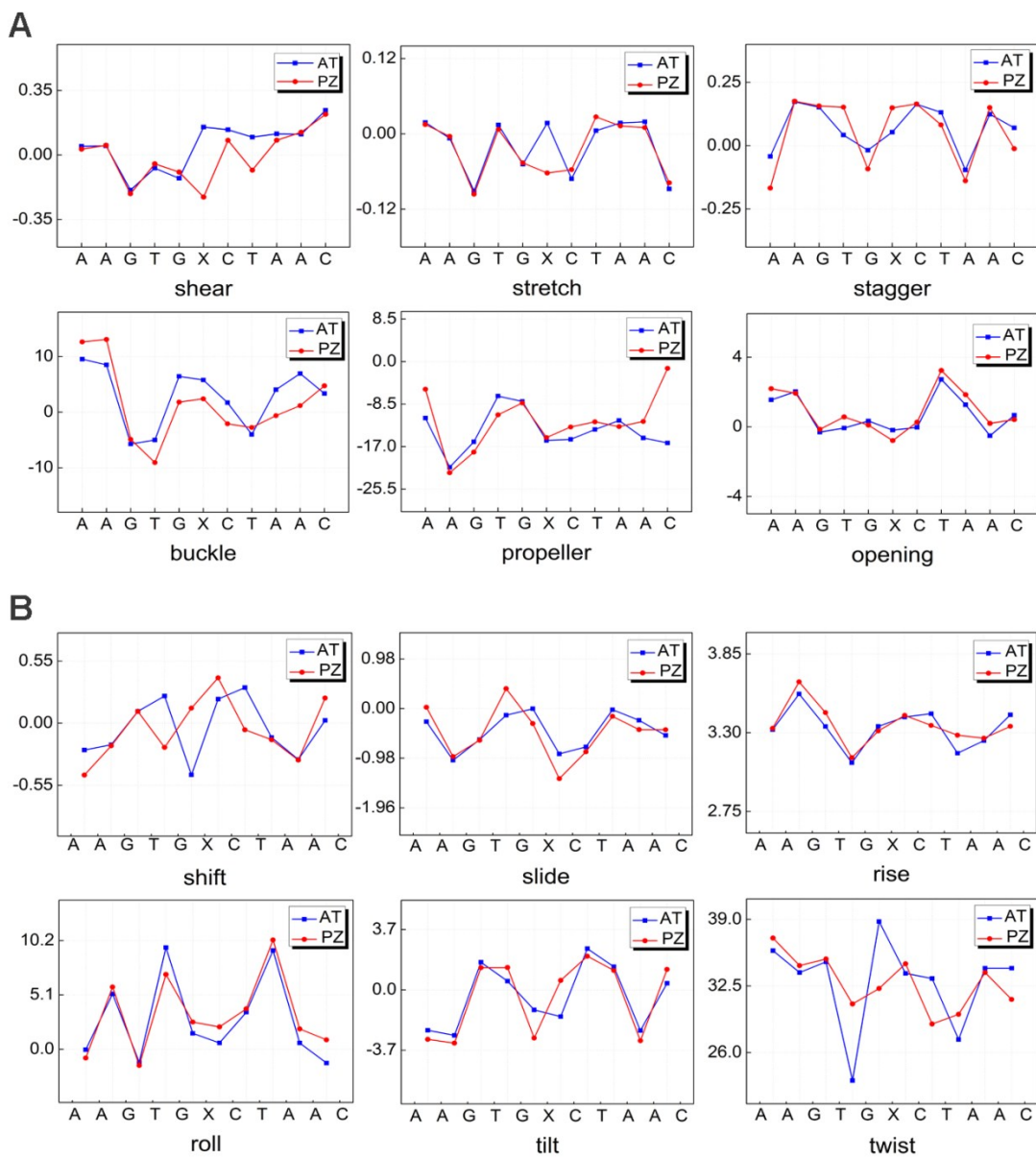


Fig. S4 Average values of the intra-base-pair (A) and inter-base-pair parameters (B) from MD simulations of oligonucleotides containing PZ^{9th} (red) and AT^{9th} (blue).

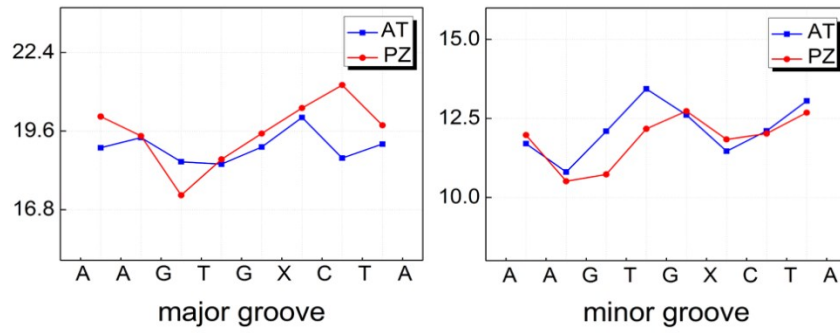


Fig. S5 Average values of groove widths parameters from MD simulations of oligonucleotides containing PZ^{9th} and AT^{9th}.

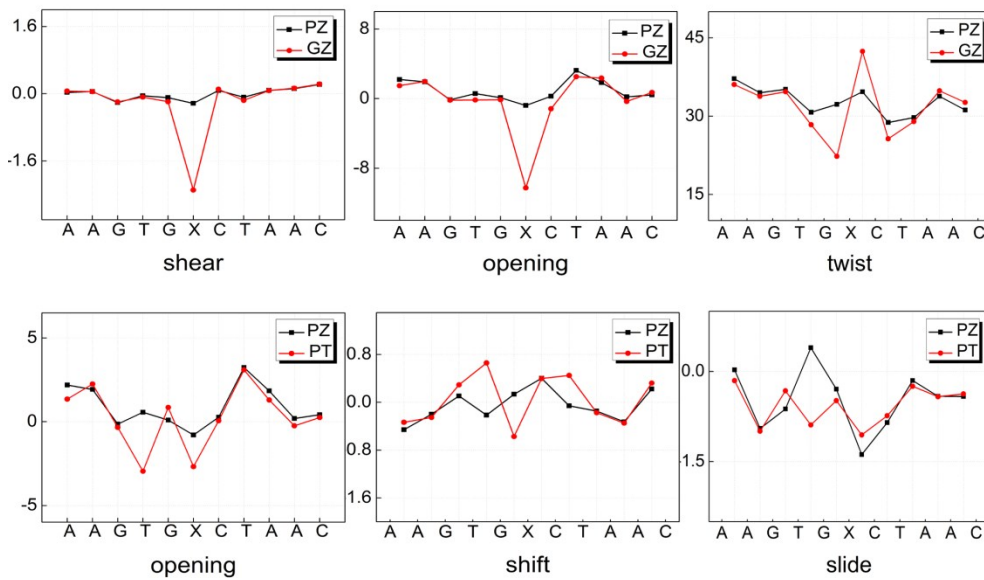


Fig. S6 Average values of intra/inter-base-pair parameters for oligonucleotides containing PZ^{9th} and mismatched PT^{9th}/GZ^{9th}, respectively.

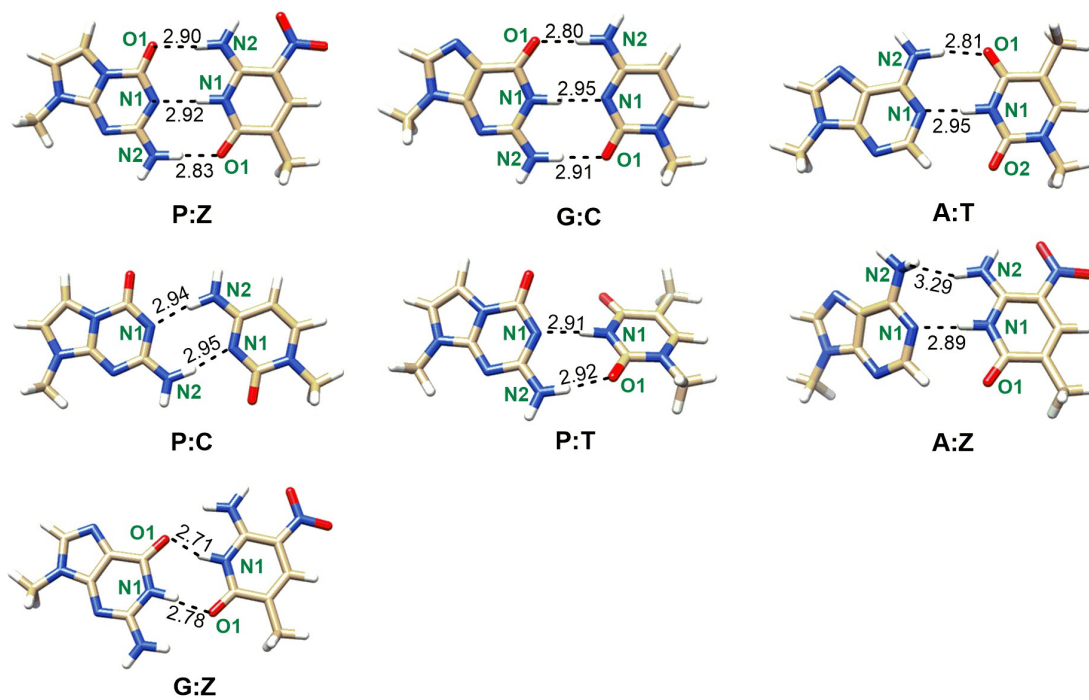


Fig. S7 The optimal geometries for the seven modeled base pairs along with H-bonding distances (in Å) in gas.

Table S1: Simulated sequences.

<i>DNA Sequence</i>	<i>X:Y pair</i>	<i>Position of the Modification</i>	<i>Duration(ns)</i>
5'-GTCAAGTG-X-CTAACG-3' 3'-CAGTTCAC-Y-GATTGC-5'	PZ	9	1500
	GC	9	1500
	AT	9	1500
	PC	9	500
	PT	9	500
	AZ	9	500
	GZ	9	500

Table S2: Energy values for gas phase interaction energy calculation of the base pairs optimized in M06-2X level.

Base Pair	E_{AB} (Hartree/ Partical)	E^0_A (Hartree/ Partical)	E^0_B (Hartree/ Partical)	ΔE_{gas} (kcal/mol)	E_{BSSE} (kcal/mol)	$E_{\text{gas.int}}$ (kcal/mol)
AT	-997.461	-505.278	-492.154	-18.077	3.897	-14.179
GC	-1013.500	-580.359	-433.093	-30.531	4.591	-25.940
PZ	-1201.550	-580.353	-621.148	-31.049	4.819	-26.231
PC	-1013.480	-580.353	-433.093	-21.679	3.778	-17.901
PT	-1072.532	-580.353	-492.154	-15.457	3.732	-11.725
AZ	-1126.452	-505.278	-621.148	-16.540	3.952	-12.588
GZ	-1201.554	-580.359	-621.148	-29.960	4.596	-25.363

Table S3: Energy values for solvent phase interaction energy calculation of the base pairs optimized in M06-2X level.

Base Pair	E_{AB} (Hartree/ Partical)	E^0_A (Hartree/ Partical)	E^0_B (Hartree/ Partical)	ΔE_{sol} (kcal/mol)	E_{BSSE} (kcal/mol)	E^{sol}_{int} (kcal/mol)
AT	-997.481	-505.291	-492.168	-13.295	3.897	-9.398
GC	-1013.527	-580.383	-433.113	-19.331	4.591	-14.740
PZ	-1201.572	-580.374	-621.166	-20.199	4.819	-15.380
PC	-1013.507	-580.374	-433.113	-12.622	3.778	-8.844
PT	-1072.562	-580.374	-492.168	-12.305	3.732	-8.573
AZ	-1126.477	-505.291	-621.166	-12.369	3.952	-8.417
GZ	-1201.576	-580.383	-621.166	-16.810	4.596	-12.213

Cartesian coordinates (Å) of gas phase optimized geometries at M06-2X/6-31G+(d,p) level.

A			O	2.2512710	-1.4922270	0.0000540	
G = -505.27813280 a.u.			C	1.2388570	0.6643090	-0.0000150	
N	-1.7822940	-0.1577220	-0.0000360	C	2.5595620	1.3706770	0.0000180
C	-1.5555030	-1.5136640	-0.0000160	C	0.0435840	1.2892250	-0.0000210
N	-0.2888710	-1.8420720	0.0000640	H	2.4223970	2.4544790	0.0000140
C	0.3618430	-0.6264970	0.0000050	H	3.1464140	1.0878300	-0.8784450
C	1.7240340	-0.2659890	-0.0000310	H	3.1463790	1.0878330	0.8785050
N	2.7071080	-1.1902070	-0.0000210	H	-0.0278430	2.3727430	0.0000310
N	2.0479190	1.0331750	-0.0000180	C	-2.4406250	1.3520480	0.0000720
C	1.0591190	1.9415260	0.0000030	H	-3.0210520	1.0861480	-0.8853090
N	-0.2552220	1.7385290	0.0000340	H	-3.0205840	1.0867000	0.8859360
C	-0.5438110	0.4313690	0.0000350	H	-2.2317580	2.4214330	-0.0003190
H	-2.3813560	-2.2137400	-0.0000470	H	-0.0556380	-2.3968570	0.0000300
H	3.6663090	-0.8839300	0.0000140				
H	1.3831560	2.9788520	0.0000130	G			
C	-3.0513290	0.5437560	-0.0000120	G = -580.35890255 a.u.			
H	-3.1291050	1.1727260	0.8890530	N	-1.9244100	-0.4041550	-0.0003190
H	-3.1284310	1.1738570	-0.8883280	C	-2.3672810	0.9022270	0.0037080
H	-3.8567200	-0.1917400	-0.0007890	N	-1.3991060	1.7775150	0.0098020
H	2.4795440	-2.1709510	0.0000290	C	-0.2550970	1.0164190	0.0105820
				C	1.1322770	1.4052220	0.0018530
T				O	1.6551380	2.4995870	-0.0080550
G = -492.15425449 a.u.				N	1.9570760	0.2371770	-0.0050430
N	-1.1703360	0.6335890	-0.0000890	C	1.5291880	-1.0631330	-0.0011550
C	-1.2472820	-0.7485640	-0.0001880	N	2.5051190	-2.0287960	-0.0658100
O	-2.3069660	-1.3466320	0.0000810	N	0.2723870	-1.4128840	0.0110640
N	-0.0202560	-1.3838550	0.0000020	C	-0.5629310	-0.3383040	0.0028190
C	1.2494690	-0.8006240	-0.0000180	H	-3.4248330	1.1313020	0.0015860

H	3.3886810	-1.8338700	0.3821600	C	1.6255960	-0.9536310	-0.0001390
H	2.1502980	-2.9609140	0.0956990	N	2.5672430	-1.9221260	-0.0013500
H	2.9460600	0.4418030	-0.0849100	N	0.3401960	-1.3978310	-0.0000640
C	-2.7142690	-1.6199340	-0.0087090	C	-0.5211490	-0.4017580	-0.0001940
H	-2.4846880	-2.2097460	-0.8983710	N	-0.1934110	0.9155340	-0.0002830
H	-2.4954380	-2.2152730	0.8800620	C	1.1908900	1.3301650	0.0001380
H	-3.7699660	-1.3469740	-0.0142370	O	1.4225320	2.5208470	0.0004650
C				C	-1.3445380	1.6897600	-0.0002400
G = -433.09259185 a.u.				C	-2.3857430	0.8260590	-0.0001270
N	-1.1095140	0.4457850	-0.0000860	N	-1.8740990	-0.4716520	-0.0002020
C	-0.6233280	-0.8959680	-0.0002780	C	-2.6311870	-1.7092940	0.0004920
O	-1.4438590	-1.7971940	0.0001470	H	2.2900950	-2.8885910	0.0039290
N	0.7323120	-1.0739720	-0.0000650	H	-1.2875070	2.7657730	-0.0003510
C	1.5394110	-0.0372890	0.0000370	H	-3.4487830	1.0066250	-0.0001990
N	2.8711310	-0.2903380	0.0002100	H	-1.9157890	-2.5317590	-0.0001060
C	1.0837000	1.3252220	0.0000040	H	-3.2553640	-1.7684500	0.8949100
C	-0.2625520	1.4991310	0.0000000	H	-3.2568630	-1.7684700	-0.8928720
H	3.5535800	0.4470630	-0.0005950	H	3.5369760	-1.6534550	0.0035000
H	1.7631130	2.1665630	0.0000920	Z			
H	-0.7212370	2.4833860	0.0000730	G = -621.14750027 a.u.			
H	3.1710020	-1.2527070	-0.0002840	N	-2.1334030	-0.7135910	-0.0000360
C	-2.5567500	0.6119500	0.0000500	C	1.5830120	-0.8172660	0.0000270
H	-2.9835490	0.1334340	-0.8832690	C	1.9154050	0.5998800	-0.0000930
H	-2.9833960	0.1334960	0.8834810	O	3.0352470	1.0806210	-0.0002060
H	-2.7890340	1.6777150	0.0000380	N	0.8065740	1.4750050	-0.0000700
P				C	-0.5118170	1.1373930	0.0000900
G = -580.35329189 a.u.				N	-1.4055410	2.1383580	0.0006300
N	2.0677510	0.3023260	0.0001690	C	-0.7949680	-0.2330790	0.0001750
				C	0.2750830	-1.1780810	0.0001610

C 2.7342320 -1.7763150 0.0000610
O -3.0620570 0.1065940 -0.0001360
O -2.3185060 -1.9211200 -0.0001910
H -1.1084310 3.1001700 -0.0022410
H -0.0073700 -2.2258920 0.0002400
H 2.3773530 -2.8078680 -0.0001110
H 3.3674780 -1.6173250 -0.8779630
H 3.3672420 -1.6175590 0.8783020
H -2.3870910 1.8931200 -0.0005430
H 1.0742530 2.4529950 0.0003770

P:Z pair

G = -1201.55027220 a.u.

N 1.3017870 0.2719550 -0.0012810
C 2.0912340 1.3692780 -0.0085810
N 1.4791040 2.5491760 -0.0140790
N 3.4500030 1.3831820 -0.0105120
C 3.9681950 0.1769300 -0.0035610
N 3.2622180 -0.9867210 0.0057310
C 1.8392340 -0.9576220 0.0058500
O 1.2413440 -2.0260700 0.0124620
C 4.1308260 -2.0717320 0.0127970
C 5.3781150 -1.5557560 0.0075280
N 5.2776870 -0.1641250 -0.0042950
C 6.3679740 0.7937640 -0.0060790
N -4.6091360 -1.7636120 -0.0058070
C -3.5690610 1.7947090 0.0064020
C -2.1273910 1.6677320 0.0052330
O -1.3502300 2.6272080 0.0070240
N -1.6188150 0.3736670 0.0018130

C -2.3412120 -0.7819910 -0.0016540
N -1.6601100 -1.9251380 -0.0046210
C -3.7426900 -0.6383130 -0.0020120
C -4.3157510 0.6596680 0.0024440
C -4.1290560 3.1844090 0.0114140
O -4.1184660 -2.8989730 -0.0099570
O -5.8170080 -1.5700390 -0.0049780
H 2.0499200 3.3776020 -0.0168510
H 3.7577500 -3.0817160 0.0199400
H 6.3387360 -2.0448910 0.0095270
H 5.9287360 1.7868320 -0.0971320
H -0.6386800 -1.9382840 0.0006390
H -5.3992940 0.7101620 0.0026240
H 6.9333150 0.7282270 0.9258270
H 7.0289980 0.6054710 -0.8540820
H -5.2204140 3.1620530 0.0124570
H -3.7850780 3.7375440 0.8904460
H -3.7868500 3.7433520 -0.8646260
H -2.2041220 -2.7759870 -0.0062980
H 0.4543900 2.6049660 -0.0075250
H -0.5841860 0.3125090 0.0013250

GC pair

G = -1013.50014902 a.u.

N -4.3693880 -0.6699380 -0.0090250
C -2.9674100 -0.7986890 -0.0018530
O -2.4923390 -1.9367690 -0.0023600
N -2.2143840 0.3283920 0.0050650
C -2.7787370 1.5348790 0.0042360
N -1.9767060 2.6001770 0.0101640

C -4.2094470 1.6928350 -0.0026900
 C -4.9487190 0.5580710 -0.0091830
 N 4.6337920 -0.3202420 -0.0125390
 C 4.9393700 1.0276190 -0.0164120
 N 3.8884970 1.7983220 -0.0102950
 C 2.8260230 0.9206410 -0.0002380
 C 1.4132730 1.1449120 0.0070540
 O 0.7978210 2.2138620 0.0077780
 N 0.7048720 -0.0653020 0.0139150
 C 1.2565510 -1.3217110 0.0134900
 N 0.3909470 -2.3540700 0.0243630
 N 2.5562480 -1.5457250 0.0062400
 C 3.2715300 -0.3993100 -0.0008490
 H -2.3657690 3.5282950 0.0083130
 H -4.6761280 2.6686020 -0.0030420
 H -6.0338120 0.5715290 -0.0149100
 H 5.9683370 1.3631300 -0.0256450
 H -0.6212910 -2.2258650 0.0129270
 H 0.7872020 -3.2786970 0.0115500
 H -0.3233510 0.0297070 0.0160680
 H -0.9512910 2.4772600 0.0113290
 C -5.1510070 -1.9015030 -0.0161500
 H -4.9051480 -2.4900740 -0.9015260
 H -4.9119220 -2.4956410 0.8673450
 H -6.2101170 -1.6424680 -0.0194110
 C 5.5439360 -1.4468990 -0.0071000
 H 5.4557940 -2.0027030 0.9292990
 H 5.3119180 -2.1150780 -0.8388350
 H 6.5624090 -1.0711120 -0.1138430

A:T pair

G = -997.46119449 a.u.

N 3.9188300 -1.2907980 0.0013090
 C 2.5302680 -1.3173240 -0.0008400
 O 1.9049210 -2.3654120 -0.0016140
 N 1.9286100 -0.0819700 -0.0021850
 C 2.5550570 1.1474540 -0.0010440
 O 1.8985350 2.1884450 -0.0020020
 C 4.0158550 1.1117930 0.0012130
 C 4.7565000 2.4136740 0.0022720
 C 4.6102250 -0.1010740 0.0022800
 N -4.8613840 -0.4017860 0.0020860
 C -5.1460850 0.9434210 0.0033480
 N -4.0858800 1.7101410 0.0021460
 C -3.0372760 0.8163410 -0.0003350
 C -1.6359760 0.9898340 -0.0020550
 N -1.0517910 2.1945750 -0.0020330
 N -0.8759990 -0.1219410 -0.0037720
 C -1.4580330 -1.3365550 -0.0035810
 N -2.7536310 -1.6174710 -0.0019810
 C -3.4943670 -0.4983850 -0.0003730
 H 5.8366000 2.2486590 0.0036000
 H 4.4886000 3.0078290 0.8806030
 H 4.4907710 3.0079870 -0.8766070
 H 5.6916770 -0.2020610 0.0040040
 H -6.1703180 1.2940070 0.0053720
 H -0.0349080 2.2780700 -0.0025250
 H -0.7631910 -2.1737680 -0.0048160
 C -5.7863390 -1.5186280 0.0024260
 H -5.6375680 -2.1263590 -0.8923950

H -5.6193680 -2.1394210 0.8849060
H -6.8045870 -1.1281520 0.0157100
C 4.5951390 -2.5827840 0.0027450
H 4.3097080 -3.1539090 0.8881970
H 4.3109540 -3.1550790 -0.8823340
H 5.6712080 -2.4099790 0.0034020
H -1.6345190 3.0164820 -0.0002150
H 0.8761910 -0.0904190 -0.0033160

P:C pair

G = -1013.48043106 a.u.

N -0.9419180 0.5724550 -0.0239970
C -1.1419690 -0.7598260 -0.0205100
N -0.0566250 -1.5325590 -0.0298950
N -2.3485450 -1.3953280 -0.0082320
C -3.3601290 -0.5580370 0.0006470
N -3.2643650 0.7995640 -0.0009220
C -1.9765660 1.4325500 -0.0130990
O -1.9279550 2.6503160 -0.0124470
C -4.5318220 1.3662130 0.0128230
C -5.4087890 0.3370400 0.0222270
N -4.6832950 -0.8544500 0.0137110
C -5.2175850 -2.2031620 0.0267680
H -0.1696220 -2.5326960 -0.0244960
H -4.6611990 2.4357810 0.0134480
H -6.4869620 0.3335730 0.0332960
H -4.3731280 -2.8908190 -0.0215190
H -5.7786850 -2.3793340 0.9474890
H -5.8660850 -2.3589310 -0.8382890
H 0.8779190 -1.1070330 -0.0328420

N 4.8849350 -0.4146770 0.0151790
C 3.5773700 -0.9646520 -0.0101340
O 3.4595980 -2.1834610 -0.0214880
N 2.5265380 -0.0999990 -0.0201390
C 2.7111970 1.2144500 -0.0047120
N 1.6269770 1.9964740 -0.0140660
C 4.0304090 1.7936410 0.0203510
C 5.0731560 0.9282060 0.0291760
H 1.7088720 2.9990440 0.0021380
H 4.1859140 2.8639420 0.0315240
H 6.1054320 1.2640830 0.0476000
H 0.6943090 1.5617450 -0.0239380
C 5.9942240 -1.3583650 0.0252180
H 5.9238070 -2.0045150 0.9022610
H 5.9528720 -1.9892740 -0.8646030
H 6.9305060 -0.7991090 0.0454070

P:T pair

G = -1072.53217860 a.u.

N -0.8695260 -0.2623260 0.5336900
C -1.4503240 -1.2936680 -0.0986100
N -0.6642810 -2.3427700 -0.3845490
N -2.7479520 -1.3909540 -0.4922650
C -3.4469000 -0.3208460 -0.1772200
N -2.9700380 0.7628430 0.4881190
C -1.5907770 0.8241670 0.8970180
O -1.2142120 1.8005160 1.5077200
C -3.9796600 1.6994030 0.6567590
C -5.0862590 1.1738010 0.0839960
N -4.7552680 -0.0796620 -0.4322510

C	-5.6343010	-0.9943210	-1.1360650	C	5.3535630	-1.1094570	-0.4178440
H	-1.0849070	-3.1475780	-0.8178380	N	4.3812520	-1.7729760	0.1534040
H	-3.7907800	2.6323990	1.1616870	C	3.3867680	-0.8303280	0.2927240
H	-6.0843320	1.5706680	-0.0105850	C	2.0999150	-0.8717980	0.8450020
H	-5.0527080	-1.8814880	-1.3864940	N	1.5450240	-2.0228090	1.3475720
H	-6.4743820	-1.2758990	-0.4973830	N	1.3629970	0.2418820	0.8372610
H	-6.0050770	-0.5305710	-2.0530140	C	1.8779870	1.3799850	0.3197980
H	0.2835810	-2.3786330	-0.0104200	N	3.0810680	1.5442160	-0.2129220
N	4.0198900	-1.0190560	0.1940570	C	3.7910280	0.4111800	-0.2044530
C	2.6438610	-1.0795920	0.2945180	H	6.3148490	-1.5265860	-0.6905400
O	2.0765280	-2.1308760	0.5893210	H	0.8928300	-1.8882040	2.1105210
N	1.9784770	0.0877260	0.0405190	H	1.2096120	2.2379980	0.3463420
C	2.5404120	1.2916130	-0.3911980	C	5.9165250	1.2242090	-1.2646710
O	1.8442530	2.2511580	-0.6635840	H	5.4236350	1.6464020	-2.1420430
C	4.0065010	1.2862310	-0.4843380	H	6.1119290	2.0220960	-0.5458980
C	4.6794840	2.5563980	-0.9027510	H	6.8561810	0.7568620	-1.5603900
C	4.6576240	0.1451270	-0.1891610	H	2.1916930	-2.7908630	1.4765070
H	5.7642960	2.4312260	-0.9427740	N	-4.3654950	-1.6593520	-0.5677650
H	4.4395680	3.3633880	-0.2044240	C	-3.3876800	1.8730690	0.0311660
H	4.3204120	2.8729050	-1.8861610	C	-1.9755520	1.7282700	0.3528840
H	5.7401800	0.0750820	-0.2392230	O	-1.2025540	2.6452060	0.6040380
C	4.7561840	-2.2509100	0.4507630	N	-1.4903310	0.4134180	0.3706370
H	4.4392670	-2.6746750	1.4043610	C	-2.1811930	-0.7150390	0.0738630
H	4.5637360	-2.9852100	-0.3355130	N	-1.5017880	-1.8739180	0.1241930
H	5.8200150	-2.0159250	0.4837300	C	-3.5399320	-0.5540380	-0.2367540
H	0.9544090	0.0629010	0.2128930	C	-4.1070570	0.7548280	-0.2441660
				C	-3.9425760	3.2650190	0.0228280
				O	-3.8726960	-2.7969580	-0.5691780
				O	-5.5406650	-1.4513220	-0.8390860
				H	-0.4940820	-1.8777120	0.2182250

A:Z pair

G = -1126.45199181 a.u.

N 5.0658000 0.2128230 -0.6623110

H	-5.1612040	0.8242510	-0.4924080	N	-3.6659080	-2.3106530	-0.0263890
H	-5.0020520	3.2572030	-0.2412830	C	-3.1066120	-1.0527330	-0.0499910
H	-3.8231400	3.7344220	1.0040990	C	-1.7498900	-0.6248700	-0.1228900
H	-3.4009250	3.8909750	-0.6928730	O	-0.7126970	-1.3060740	-0.1781350
H	-1.9967890	-2.7124370	-0.1483130	N	-1.6505620	0.7673820	-0.1237430
H	-0.4956920	0.3318120	0.6391290	C	-2.6976330	1.6449830	-0.0422600

G:Z pair

G = -1201.55414663 a.u.

N	5.1013100	-1.3581670	0.0787220	C	-4.0924370	-0.0672440	0.0256900
C	3.1868450	1.8331040	0.0298870	H	-5.7175730	-2.8455520	0.0996770
C	1.8337990	1.3358100	-0.0463440	H	-1.3899730	3.2321930	0.0239110
O	0.8150270	2.0515840	-0.0794350	H	-3.0825400	3.6258490	0.1264130
N	1.6811830	-0.0380050	-0.0859420	H	-0.7008810	1.1798620	-0.1555040
C	2.6685470	-0.9711170	-0.0471880	C	-6.5881900	-0.1433980	0.2041520
N	2.2665630	-2.2461100	-0.0882270	H	-6.7079540	0.3324480	1.1799790
C	3.9818060	-0.4801190	0.0297040	H	-6.7163190	0.6076650	-0.5770420
C	4.2007410	0.9212060	0.0643120	H	-7.3384510	-0.9255900	0.0846720
C	3.3805350	3.3192500	0.0662650				
O	4.8945510	-2.5762780	0.0488460	PZ//CG			
O	6.2215970	-0.8739710	0.1490900	C	-5.4474970	-0.8647130	1.6632250
H	1.2760190	-2.4560320	-0.1320660	N	-4.3592230	-1.6735460	1.1454390
H	5.2337100	1.2501840	0.1214830	C	-4.4307080	-2.9196740	0.5530820
H	4.4428350	3.5677730	0.1080190	N	-3.2644510	-3.4187090	0.2498280
H	2.9424950	3.7887580	-0.8197670	C	-2.3676430	-2.4572330	0.6632790
H	2.8825800	3.7553140	0.9377630	C	-0.9436430	-2.3864860	0.5572020
H	2.9664750	-2.9729810	-0.0591080	O	-0.1564740	-3.2144860	0.0884260
H	0.7105750	-0.4174170	-0.1379340	N	-0.4525930	-1.1765530	1.0674690
N	-5.2727320	-0.7439960	0.0925660	C	-1.2052020	-0.1682420	1.6139380
C	-4.9467980	-2.0868260	0.0585160	N	-0.5273120	0.9243070	2.0220790
				N	-2.5185490	-0.2134650	1.7113160

C	-3.0314660	-1.3662160	1.2204900	H	0.4886500	0.9315330	2.1047880
C	-4.0164130	4.1732800	0.7536820	H	-3.6250260	5.0650430	0.2546210
C	-4.4517770	1.9920740	-0.4532900	H	-5.5245740	2.1165880	-0.3421600
C	-4.0118690	0.8122130	-1.1097810	H	-1.0480190	-0.5785200	-1.9087340
C	-2.6291190	0.5917540	-1.2964270	H	6.8288490	0.5625880	-0.5914250
N	-2.0644330	-0.4648150	-1.8726020	H	5.8411660	-1.0854250	-2.8064060
N	-1.7976440	1.5712020	-0.8385180	H	2.1742100	3.6574890	0.6659270
C	-2.1732510	2.7027090	-0.1293680	H	4.6776120	1.2610320	3.5535800
O	-1.2983050	3.4573890	0.3165710	H	6.2939680	-0.8985200	1.5115230
C	6.1895620	1.2173620	-1.1905000	H	5.2798040	-2.8350180	0.2969880
N	4.9997100	0.5055920	-1.6109310	H	3.1279380	-3.7864150	-0.4575260
C	4.9435200	-0.6372370	-2.4108950	H	-5.1055920	4.2413810	0.7980840
C	1.5041360	0.0271030	-1.6214920	H	-3.6204190	4.1833340	1.7742030
O	0.7933060	-0.8500660	-2.0957930	H	-6.3343890	-1.0199040	1.0475630
N	1.1015430	1.0989420	-0.9196170	H	-5.6566460	-1.1196390	2.7058860
C	2.0008290	1.9703090	-0.4173720	H	6.1281830	1.0816560	2.5208410
N	1.5207690	3.0237740	0.2362440	H	4.7346040	2.0698270	1.9750160
N	3.3575850	1.8738910	-0.5243850	H	6.7452850	1.5742200	-2.0606090
C	3.7379640	0.8551710	-1.2619920	H	5.8699190	2.0694390	-0.5892230
C	5.0412540	1.1781920	2.5282500	N	2.9087070	-0.0562440	-1.8391140
N	4.4634910	0.0033850	1.8875850	C	3.6465330	-0.9913260	-2.5534210
C	5.2219180	-0.9921570	1.3642380	H	0.5080280	3.1615070	0.3285870
C	4.6695590	-2.0401070	0.7047100	H	3.1584400	-1.7999380	-3.0724460
C	3.2343040	-2.0410370	0.5769910	N	-4.9749780	-0.1504370	-1.4933730
N	2.6057140	-3.0045990	-0.0965080	O	-6.1610360	0.0724980	-1.2482550
N	2.4933160	-1.0688080	1.1068410	O	-4.6029220	-1.1924670	-2.0459330
C	3.0568240	-0.0473210	1.7992680	H	-2.6718490	-1.2273840	-2.1431230
O	2.4087300	0.8491710	2.3392500	H	-0.7759020	1.4056950	-0.8845920
H	-5.1489990	0.1842410	1.6058260	H	1.5680950	-3.0463210	-0.0968790
H	-5.3877240	-3.3853070	0.3582330	H	0.5714050	-1.0684380	1.0391580

H	-1.0656420	1.6680010	2.4376950	C	-1.5669830	-1.3234650	1.4023160
C	-3.5943700	2.9288380	0.0325520	O	-0.8445050	-2.3180700	1.3812900
				N	-1.0041620	-0.0403390	1.4389370
GC//CG				C	-1.6964020	1.1429640	1.3989880
C	5.9746410	0.7663860	-1.4050710	N	-0.9632220	2.2683460	1.4210000
N	4.9416310	-0.2454700	-1.3827100	N	-3.0189070	1.2146290	1.3609080
C	5.0887070	-1.6188380	-1.3650290	C	-3.5953910	-0.0058210	1.3852260
N	3.9524210	-2.2606910	-1.3628160	C	-4.5383920	2.5376600	-1.6431210
C	3.0006360	-1.2641960	-1.3906830	N	-3.9284140	1.2183740	-1.7364380
C	1.5670130	-1.3248000	-1.4012440	C	-4.6639650	0.0771620	-1.8094020
O	0.8445670	-2.3194160	-1.3794630	C	-4.0834850	-1.1448260	-1.7940780
N	1.0041550	-0.0417280	-1.4388750	C	-2.6504250	-1.1795080	-1.6622470
C	1.6963570	1.1416360	-1.3998860	N	-2.0121220	-2.3464240	-1.5783950
N	0.9631230	2.2669550	-1.4227960	N	-1.9287010	-0.0570120	-1.6309770
N	3.0188580	1.2133790	-1.3618940	C	-2.5277890	1.1590150	-1.6514740
C	3.5953780	-0.0070760	-1.3852000	O	-1.9055060	2.2251480	-1.5897770
C	4.5383220	2.5392290	1.6410490	H	5.9394050	1.3706750	-0.4938710
N	3.9284120	1.2199800	1.7352750	H	6.0715800	-2.0729350	-1.3622340
C	4.6639890	0.0788490	1.8092170	H	-0.0598720	2.2483920	-1.4019320
C	4.0835190	-1.1431610	1.7950040	H	4.1186820	3.1957600	2.4042600
C	2.6504630	-1.1779830	1.6632150	H	5.7398630	0.2114560	1.8775780
N	2.0121820	-2.3449840	1.5803580	H	4.6697660	-2.0507370	1.8407890
N	1.9287120	-0.0555320	1.6309620	H	0.9978060	-2.3615990	1.4205540
C	2.5277760	1.1605240	1.6504200	H	-5.9430930	1.3675450	0.4902040
O	1.9054790	2.2265960	1.5878890	H	-6.0715220	-2.0718000	1.3642920
C	-5.9746600	0.7676130	1.4044290	H	-1.4539080	3.1208960	1.2048300
N	-4.9416430	-0.2442620	1.3831530	H	-4.1184100	3.1938110	-2.4064630
C	-5.0886700	-1.6176520	1.3665200	H	-5.7398340	0.2097120	-1.8779380
N	-3.9523600	-2.2594640	1.3647080	H	-4.6697180	-2.0524490	-1.8391200
C	-3.0006060	-1.2629150	1.3916940	H	-2.5401320	-3.1800880	-1.3704100

H	-5.6153580	2.4359240	-1.7895650	C	-4.9649940	0.8903730	-1.5449140
H	-4.3262790	2.9639880	-0.6580480	C	-1.3880350	0.6751260	-1.5130890
H	6.9461320	0.2749260	-1.4781410	O	-1.0157960	-0.2896450	-2.1706280
H	5.8340700	1.4265500	-2.2637800	N	-0.6026750	1.5344160	-0.8404360
H	5.6153590	2.4375790	1.7870400	C	-1.1417170	2.5504410	-0.1339190
H	4.3257350	2.9650980	0.6558820	N	-0.2914130	3.3637570	0.4930970
H	-6.9458470	0.2765360	1.4836640	N	-2.4665530	2.8127560	0.0094820
H	-5.8306550	1.4318360	2.2593980	C	-3.2255460	1.9692530	-0.6571630
H	-0.9977380	-2.3629060	-1.4186110	C	5.3317370	3.0274830	-0.5245210
H	1.4537890	3.1197600	-1.2075990	C	4.8895170	0.5966150	-1.0759290
H	0.0597670	2.2497830	1.3999620	C	4.0126240	-0.4875250	-1.3576320
H	2.5402090	-3.1788060	1.3730550	C	2.6163600	-0.2598520	-1.4355600
H	0.0309700	-0.0133000	1.4702530	N	1.6843090	-1.1430690	-1.7670400
H	-0.0309770	-0.0147480	-1.4702070	N	2.2013380	1.0012420	-1.1249510
				C	3.0079410	2.0681880	-0.7511470
GC/PZ				O	2.4849140	3.1247170	-0.3845960
C	-6.3288560	-0.8716330	1.1233920	C	3.9578780	1.4785030	2.4818410
N	-5.1967250	-1.5592220	0.5448430	N	3.4248350	0.1871190	2.0564450
C	-5.2002990	-2.6361790	-0.3213670	C	4.2230710	-0.9035620	1.9001200
N	-4.0041060	-3.0485910	-0.6378380	C	3.7267470	-2.0996130	1.5020630
C	-3.1597560	-2.2029880	0.0474580	C	2.3206630	-2.1466940	1.2114500
C	-1.7280220	-2.1707460	0.1532320	N	1.7598450	-3.2611370	0.7312900
O	-0.8933590	-2.9282350	-0.3381310	N	1.5363910	-1.0869630	1.4078090
N	-1.3097720	-1.1063450	0.9668400	C	2.0425590	0.0948790	1.8378190
C	-2.1199070	-0.2049940	1.6048130	O	1.3458620	1.0992250	2.0260560
N	-1.4994780	0.7364410	2.3464770	H	-6.2810570	0.1950490	0.8862940
N	-3.4411440	-0.2340520	1.5341750	H	-6.1303290	-3.0705420	-0.6654990
C	-3.8844470	-1.2627660	0.7755420	H	-0.4978720	0.9157920	2.2244840
C	-5.4166640	2.8426320	0.0477390	H	-5.0436650	3.8640350	-0.0398630
N	-4.5728920	1.9575360	-0.7328560	H	-6.0067080	0.6863140	-1.7370400

H	0.7140480	3.2547470	0.3497180	GC//GC			
H	5.0989840	3.4712620	0.4490890	C	4.5238170	-2.1423770	-1.1340930
H	5.9523450	0.3746990	-1.0767270	N	3.1587840	-2.6327200	-1.2203680
H	1.9746440	-2.0932130	-1.9465630	C	2.7004200	-3.8847220	-0.8823850
H	3.7198280	1.6590420	3.5334350	N	1.3964820	-3.9842100	-0.8741120
H	5.2807410	-0.7487400	2.0882790	C	0.9681580	-2.7185530	-1.2147590
H	4.3745700	-2.9502740	1.3333030	C	-0.3399130	-2.1553190	-1.2464660
H	2.3604850	-4.0018250	0.4025970	O	-1.4266140	-2.7213710	-1.0579860
H	3.5032770	2.2680980	1.8809890	N	-0.3049400	-0.7800050	-1.4854790
H	5.0391360	1.4725980	2.3343650	C	0.8285370	-0.0335730	-1.6868260
H	6.3824830	2.7285380	-0.5381360	N	0.6363210	1.2897390	-1.9291520
H	5.1810150	3.8161920	-1.2682660	N	2.0417000	-0.5386930	-1.6790370
H	-7.2457430	-1.2958090	0.7109040	C	2.0501460	-1.8640700	-1.4114830
H	-6.3305650	-0.9860320	2.2098670	C	5.1440380	3.9664100	-0.3044200
H	-6.4336070	2.7884250	-0.3420790	N	4.8767920	2.6161050	0.1459530
H	-5.3992060	2.5431100	1.0997590	C	5.7663720	1.5697400	0.2870290
H	-2.0863770	1.4936060	2.6613000	N	5.2066180	0.4685560	0.7061460
H	-0.2813150	-1.0389000	1.1010490	C	3.8762820	0.7986090	0.8556590
H	0.7995060	-3.2133850	0.3723220	C	2.7403360	0.0091920	1.2248620
H	1.1768590	1.1878690	-1.0503820	O	2.6903870	-1.1992470	1.4675190
H	0.6958640	-0.8793160	-1.8371170	N	1.5735840	0.7846310	1.2771310
N	4.5575970	-1.7855480	-1.4317730	C	1.4753000	2.1093940	0.9310930
O	5.7616090	-1.9344650	-1.2318750	N	0.2607610	2.6742310	1.0482940
O	3.8037030	-2.7486010	-1.6454380	N	2.5001320	2.8292160	0.5047900
H	-0.6638050	4.1606960	0.9823500	C	3.6545710	2.1268030	0.5091270
N	-2.7789230	0.9361750	-1.4237100	C	-4.5010840	0.0900250	2.0975670
C	-3.8561210	0.2516050	-1.9779880	N	-3.2853630	-0.6970530	1.9623050
H	-3.7095010	-0.6247640	-2.5899790	C	-3.3086220	-2.0600760	1.9639610
C	4.4446080	1.8526440	-0.8079940	C	-2.1733830	-2.7852180	1.8831440
				C	-0.9388400	-2.0494750	1.8019060

N	0.2252640	-2.7003760	1.7635440	H	-6.2725360	2.3137980	-1.1498220
N	-0.9191850	-0.7159990	1.7860060	H	-6.2839500	-0.1700750	-1.4337610
C	-2.0717170	-0.0025930	1.8503230	H	-4.8151310	-2.1715450	-1.4283640
O	-2.1103270	1.2328220	1.8180810	H	-5.3608440	-0.5546530	1.9058410
C	-4.1873080	3.8698560	-0.7916010	H	-4.5719340	0.5192310	3.1011290
N	-4.2083550	2.4217290	-0.9657040	H	5.2057020	-2.9088640	-1.5075160
C	-5.3594450	1.7269920	-1.1454080	H	4.6026820	-1.2465260	-1.7513040
C	-5.3619120	0.3790450	-1.2969760	H	6.2234740	4.0983560	-0.3910930
C	-4.0837160	-0.2786350	-1.2243170	H	4.6764280	4.1451070	-1.2757200
N	-3.9959140	-1.6134320	-1.2534050	H	-3.6372430	4.1130210	0.1189420
N	-2.9547760	0.4112420	-1.1018980	H	-5.2144400	4.2281250	-0.7161610
C	-2.9603500	1.7672050	-1.0276800	H	1.4720730	1.8512440	-1.8350510
O	-1.9410830	2.4547290	-1.0166010	H	-1.2161930	-0.3034340	-1.3990790
H	4.7639140	-1.8745300	-0.1026240	H	0.1500390	3.5794240	0.6199940
H	3.3919590	-4.6860210	-0.6564490	H	0.7044150	0.2758610	1.5164370
H	-0.2315750	1.7210310	-1.6085140	H	1.0970980	-2.1705340	1.6526380
H	4.7446270	4.6813400	0.4173810	H	-3.0648070	-2.0606460	-1.2055110
H	6.8181960	1.7006580	0.0682660				
H	-0.5830610	2.1263480	1.2369300				
H	-4.4802330	0.9085790	1.3774520				
H	-4.2911290	-2.5160090	2.0294040				
H	-2.1873460	-3.8658230	1.8524050				
H	0.2393130	-3.6731520	1.4890330				
H	-3.6838760	4.3415550	-1.6376320				

Cartesian coordinates (Å) of solvent phase optimized geometries at M06-2X/6-31G+(d,p) level.

A				O	2.2505970	-1.4987350	0.0002280
G = -505.29145873 a.u.				C	1.2379210	0.6599570	-0.0001040
N	-1.7828780	-0.1552020	-0.0000330	C	2.5521180	1.3799490	-0.0000200
C	-1.5627740	-1.5076210	-0.0000450	C	0.0394670	1.2856820	-0.0000990
N	-0.2927000	-1.8397630	0.0000800	H	2.3991640	2.4608400	0.0000160
C	0.3627960	-0.6264840	0.0000020	H	3.1415490	1.1104710	-0.8812830
C	1.7286370	-0.2722310	-0.0000330	H	3.1414810	1.1104030	0.8812670
N	2.7104210	-1.1915160	-0.0000110	H	-0.0327120	2.3682230	-0.0000320
N	2.0508910	1.0327900	-0.0000220	C	-2.4390440	1.3580170	0.0000660
C	1.0633450	1.9430200	0.0000010	H	-3.0155660	1.0988680	-0.8889780
N	-0.2505770	1.7400780	0.0000280	H	-3.0153460	1.0988310	0.8892460
C	-0.5451860	0.4302880	0.0000280	H	-2.2218570	2.4243610	0.0000600
H	-2.3917590	-2.2033560	-0.0000750	H	-0.0526880	-2.3966710	0.0001820
H	3.6743700	-0.8951900	0.0000260				
H	1.3885700	2.9802440	0.0000010	G			
C	-3.0588830	0.5420970	0.0000020	G = -580.38332773 a.u.			
H	-3.1397940	1.1656660	0.8917760	N	-1.9250280	-0.4031850	0.0001630
H	-3.1391450	1.1668070	-0.8910250	C	-2.3651070	0.8996220	0.0011330
H	-3.8584600	-0.1977040	-0.0007730	N	-1.3917180	1.7757880	0.0028490
H	2.4925040	-2.1755970	0.0000500	C	-0.2474370	1.0077430	0.0024910
				C	1.1333390	1.3847670	0.0010660
T				O	1.6366190	2.5048710	-0.0003740
G = -492.16844063 a.u.				N	1.9608590	0.2433580	-0.0023890
N	-1.1703410	0.6290820	-0.0001240	C	1.5390640	-1.0641420	-0.0001440
C	-1.2401950	-0.7453040	-0.0002360	N	2.5029510	-2.0189210	-0.0567940
O	-2.3006660	-1.3578420	0.0002590	N	0.2730160	-1.4122730	0.0050500
N	-0.0172640	-1.3827160	-0.0000520	C	-0.5631840	-0.3462360	0.0004280
C	1.2446940	-0.7961790	-0.0001310	H	-3.4223220	1.1290880	0.0006250

H	3.4424260	-1.8028580	0.2436850	C	2.1219950	1.3991100	-0.0043200
H	2.1898110	-2.9615900	0.1269310	N	1.5195930	2.5917090	-0.0084320
H	2.9551150	0.4431750	-0.0274730	N	3.4708900	1.3901490	-0.0072580
C	-2.7294750	-1.6149830	-0.0012730	C	3.9831000	0.1723110	-0.0039060
H	-2.5076520	-2.2056430	-0.8914210	N	3.2532200	-0.9795080	0.0043420
H	-2.5131700	-2.2044270	0.8910730	C	1.8432650	-0.9202780	0.0070730
H	-3.7809190	-1.3307100	-0.0047770	O	1.2100040	-1.9799950	0.0133730
C				C	4.1092480	-2.0789110	0.0078320
G = -433.11300410 a.u.				C	5.3633990	-1.5751380	0.0011410
N	-1.1119300	0.4360810	0.0000060	N	5.2806390	-0.1845740	-0.0081870
C	-0.6219260	-0.8833540	-0.0000020	C	6.4019420	0.7454480	-0.0051290
O	-1.4389110	-1.8102640	-0.0000020	N	-4.5890380	-1.7745540	-0.0062000
N	0.7244090	-1.0756730	-0.0000480	C	-3.5985010	1.7855490	0.0029370
C	1.5478480	-0.0345910	-0.0000320	C	-2.1529920	1.6668940	0.0057350
N	2.8697310	-0.2852890	0.0000990	O	-1.3785500	2.6316350	0.0087810
C	1.0832090	1.3202400	0.0000240	N	-1.6270290	0.3818700	0.0047660
C	-0.2624770	1.4935660	0.0000290	C	-2.3353800	-0.7820540	0.0009850
H	3.5473760	0.4600500	-0.0005020	N	-1.6403190	-1.9125030	0.0005100
H	1.7619200	2.1618460	0.0000690	C	-3.7459860	-0.6523330	-0.0020660
H	-0.7219750	2.4760230	0.0000590	C	-4.3344710	0.6442420	-0.0009050
H	3.1935630	-1.2405910	-0.0004170	C	-4.1831760	3.1658000	0.0039450
C	-2.5606440	0.6206090	0.0000310	O	-4.0938330	-2.9144960	-0.0082030
H	-2.9930010	0.1557690	-0.8872520	O	-5.8114240	-1.6058190	-0.0078520
H	-2.9929550	0.1559660	0.8874410	H	2.0877140	3.4244090	-0.0117330
H	-2.7751790	1.6884070	-0.0000820	H	3.7352760	-3.0887530	0.0134230
P:Z pair				H	6.3190710	-2.0752940	0.0001500
G = -1201.57225383 a.u.				H	6.0027840	1.7512990	-0.1248180
N	1.3117210	0.3109620	0.0025580	H	-0.6137390	-1.9061610	0.0049870
				H	-5.4179850	0.6939640	-0.0033660
				H	6.9411220	0.6720670	0.9402830

H 7.0682740 0.5115800 -0.8356230
H -5.2736120 3.1177440 0.0016480
H -3.8581860 3.7265110 0.8857530
H -3.8546140 3.7292480 -0.8748020
H -2.1514070 -2.7836420 -0.0021390
H 0.5018000 2.6532520 -0.0027260
H -0.5884760 0.3344830 0.0055450

G:C pair

G = -1013.52713785 a.u.

N -4.3550930 -0.6911420 -0.0186640
C -2.9637380 -0.7909280 -0.0764520
O -2.4571520 -1.9218710 -0.1630410
N -2.2201100 0.3420740 -0.0377030
C -2.8087930 1.5386760 0.0589210
N -2.0232640 2.6189320 0.0902640
C -4.2337120 1.6703350 0.1266730
C -4.9556490 0.5239490 0.0826660
N 4.6368770 -0.3354010 0.0196690
C 4.9551910 1.0022970 -0.0433680
N 3.9066310 1.7839890 -0.0869430
C 2.8359400 0.9135700 -0.0504000
C 1.4294070 1.1516710 -0.0684350
O 0.8376860 2.2397420 -0.1216910
N 0.7011490 -0.0378320 -0.0172850
C 1.2398510 -1.3014680 0.0494060
N 0.3636510 -2.3189810 0.1155700
N 2.5402370 -1.5383470 0.0675900
C 3.2744760 -0.4059930 0.0167250
H -2.4270850 3.5400200 0.1591070

H -4.7142410 2.6357280 0.2069600
H -6.0390020 0.5169760 0.1248640
H 5.9872660 1.3270200 -0.0541180
H -0.6434830 -2.1764060 -0.0004250
H 0.7412070 -3.2534170 0.0903560
H -0.3307610 0.0689380 -0.0289270
H -1.0079890 2.5164060 0.0206450

C -5.1306010 -1.9298580 -0.0621210

H -4.9106380 -2.4698400 -0.9837950

H -4.8689950 -2.5592550 0.7894990

H -6.1886390 -1.6759440 -0.0245930

C 5.5506980 -1.4638800 0.0890260

H 5.4263050 -1.9881370 1.0381980

H 5.3527950 -2.1509870 -0.7350480

H 6.5700230 -1.0873290 0.0117880

A:T pair

G = -997.48108677 a.u.

N 3.9437170 -1.2852150 0.0083180
C 2.5652080 -1.3166710 -0.0041460
O 1.9288950 -2.3665430 -0.0084570
N 1.9534440 -0.0868550 -0.0115470
C 2.5734350 1.1455700 -0.0058390
O 1.8956490 2.1801800 -0.0120180
C 4.0266240 1.1194020 0.0075570
C 4.7730610 2.4189440 0.0136540
C 4.6281810 -0.0929430 0.0139110
N -4.8851890 -0.3994220 0.0144280
C -5.1678620 0.9416530 0.0222540
N -4.1023610 1.7083340 0.0133610

C	-3.0546920	0.8130000	-0.0020180	N	-2.3605680	-1.3908450	0.0024280
C	-1.6530380	0.9828550	-0.0136870	C	-3.3870980	-0.5586510	0.0110460
N	-1.0583360	2.1824760	-0.0146710	N	-3.2903030	0.8000650	-0.0232860
N	-0.8927440	-0.1313080	-0.0248260	C	-2.0149470	1.4252740	-0.0746450
C	-1.4801100	-1.3413060	-0.0238150	O	-1.9603540	2.6515510	-0.1018260
N	-2.7764200	-1.6202260	-0.0131860	C	-4.5634490	1.3627130	0.0041100
C	-3.5207150	-0.4999180	-0.0020130	C	-5.4310990	0.3273090	0.0537860
H	5.8507130	2.2443740	0.0210360	N	-4.7002510	-0.8583490	0.0548750
H	4.5097440	3.0135310	0.8933980	C	-5.2466060	-2.2062720	0.1243780
H	4.5218610	3.0144970	-0.8689650	H	-0.1744680	-2.5225480	-0.0201940
H	5.7090510	-0.1884610	0.0241620	H	-4.7115590	2.4291440	-0.0170270
H	-6.1916820	1.2920690	0.0355760	H	-6.5089380	0.3161720	0.0862130
H	-0.0405820	2.2511300	-0.0160570	H	-4.4303350	-2.9088670	-0.0360750
H	-0.7899830	-2.1823180	-0.0324410	H	-5.6923350	-2.3773570	1.1055470
C	-5.8275010	-1.5074000	0.0145740	H	-5.9993410	-2.3328560	-0.6540870
H	-5.7420150	-2.0702210	-0.9163600	H	0.8593920	-1.0877340	-0.0791200
H	-5.6202520	-2.1648830	0.8599620	N	4.9114690	-0.4211690	0.0367880
H	-6.8348580	-1.1031180	0.1058450	C	3.6169450	-0.9576600	-0.0581360
C	4.6411550	-2.5707480	0.0162540	O	3.4868480	-2.1848160	-0.1308930
H	4.3647520	-3.1378790	0.9062600	N	2.5606510	-0.1027550	-0.0664400
H	4.3714430	-3.1444360	-0.8715180	C	2.7465490	1.2148860	0.0198030
H	5.7126920	-2.3805150	0.0195460	N	1.6605300	1.9974200	0.0094570
H	-1.6218930	3.0185110	-0.0004260	C	4.0575590	1.7876970	0.1179390
H	0.9074080	-0.1004790	-0.0194700	C	5.1007070	0.9212910	0.1217630
P:C pair				H	1.7517640	2.9986060	0.0815900
G	= -1013.50725843 a.u.			H	4.2119380	2.8557540	0.1864820
N	-0.9685990	0.5813800	-0.0883670	H	6.1307140	1.2536240	0.1915420
C	-1.1672500	-0.7551600	-0.0483860	H	0.7298420	1.5696820	-0.0417340
N	-0.0693830	-1.5209840	-0.0615860	C	6.0344490	-1.3549630	0.0419970
				H	5.9516550	-2.0305260	0.8947930

H 6.0305020 -1.9441650 -0.8760530
H 6.9598240 -0.7849260 0.1108490

P:T pair

G = -1072.56218909 a.u.

N -0.8891660 -0.2054170 0.4893510
C -1.4578750 -1.2603150 -0.1362020
N -0.6462240 -2.2890580 -0.4270270
N -2.7494650 -1.3804970 -0.5089090
C -3.4775100 -0.3240100 -0.1880130
N -3.0071540 0.7764080 0.4613760
C -1.6377040 0.8617220 0.8331970
O -1.2515100 1.8654480 1.4210930
C -4.0402630 1.6913520 0.6433840
C -5.1410220 1.1289640 0.0959580
N -4.7885830 -0.1173250 -0.4163400
C -5.6776530 -1.0530840 -1.0908000
H -1.0483090 -3.1202370 -0.8317270
H -3.8799200 2.6352280 1.1364800
H -6.1518940 1.4967020 0.0190390
H -5.1005430 -1.9410010 -1.3437420
H -6.4980830 -1.3234550 -0.4250940
H -6.0699220 -0.5972020 -2.0008080
H 0.2959830 -2.3118790 -0.0424160
N 4.0291270 -1.0496340 0.1906450
C 2.6654910 -1.0673370 0.3457680
O 2.0617320 -2.0853550 0.6934500
N 2.0197790 0.1144370 0.0866700
C 2.6047510 1.2985470 -0.3460160
O 1.9122910 2.2870750 -0.5737330

C 4.0541650 1.2545080 -0.4955060
C 4.7625750 2.4960390 -0.9445780
C 4.6831780 0.0911720 -0.2194920
H 5.8366520 2.3193000 -1.0273540
H 4.5959800 3.3139420 -0.2372350
H 4.3859950 2.8257610 -1.9172730
H 5.7597460 -0.0088610 -0.3108320
C 4.7500870 -2.2950570 0.4559630
H 4.5699780 -2.6149820 1.4830170
H 4.4093850 -3.0742960 -0.2274760
H 5.8128840 -2.1142070 0.3073850
H 0.9944470 0.1004300 0.2392270

A:Z pair

G = -1126.47709443 a.u.

N 4.9062770 0.0951760 -0.8333670
C 5.1720880 -1.1851310 -0.4211840
N 4.2361440 -1.7086490 0.3349240
C 3.2921120 -0.7090750 0.4232320
C 2.0615580 -0.6079280 1.0898720
N 1.5044300 -1.6361540 1.7991640
N 1.3656260 0.5307840 0.9733430
C 1.8681100 1.5444150 0.2408320
N 3.0181650 1.5736430 -0.4169990
C 3.6924710 0.4208680 -0.2968060
H 6.0871730 -1.6819110 -0.7168860
H 0.9238080 -1.3630420 2.5843130
H 1.2374480 2.4287590 0.1894010
C 5.7357820 0.9522880 -1.6674230
H 5.1830130 1.2413810 -2.5621700

H	6.0239180	1.8440740	-1.1091600	C	2.7157920	-0.9830170	-0.0346410
H	6.6270900	0.3952110	-1.9526050	N	2.3316080	-2.2586810	-0.0579520
H	2.1137550	-2.4211740	1.9936660	C	4.0316100	-0.4786490	0.0245840
N	-4.1035370	-1.7952150	-0.6793480	C	4.2413860	0.9289560	0.0389110
C	-3.4249160	1.7828710	-0.0346940	C	3.4053210	3.3163030	0.0152640
C	-2.0481020	1.7240240	0.4308210	O	4.9620610	-2.5658740	0.0586370
O	-1.3666680	2.6981070	0.7494020	O	6.2743230	-0.8522850	0.1306620
N	-1.4777450	0.4537430	0.5142850	H	1.3457320	-2.4867020	-0.0944040
C	-2.0564970	-0.7238620	0.1667790	H	5.2694550	1.2731160	0.0815710
N	-1.3195370	-1.8272580	0.2837670	H	4.4660260	3.5700990	0.0538610
C	-3.3926490	-0.6491080	-0.2925220	H	2.9679600	3.7695490	-0.8795960
C	-4.0379070	0.6207110	-0.3755350	H	2.9057410	3.7626480	0.8804840
C	-4.0714640	3.1326180	-0.1144740	H	3.0293900	-2.9872460	-0.0297580
O	-3.5568720	-2.9100100	-0.6074350	H	0.7497850	-0.4260440	-0.1118960
O	-5.2623440	-1.6737930	-1.0843800	N	-5.3060910	-0.7765750	0.0619620
H	-0.3734030	-1.7994430	0.6528830	C	-4.9584790	-2.1077360	0.0191270
H	-5.0627330	0.6283800	-0.7308670	N	-3.6669720	-2.3074120	-0.0451680
H	-5.0936370	3.0461450	-0.4873870	C	-3.1313250	-1.0363790	-0.0440750
H	-4.0953200	3.6115720	0.8694130	C	-1.7839870	-0.5840370	-0.0919510
H	-3.5083860	3.7940220	-0.7801520	O	-0.7414220	-1.2642140	-0.1459090
H	-1.7402960	-2.7131530	0.0417370	N	-1.7014430	0.8052310	-0.0709870
H	-0.4876260	0.4561230	0.8233410	C	-2.7669110	1.6660170	-0.0015860

G:Z pair

G = -1201.57604085 a.u.

N	5.1452230	-1.3389800	0.0734640	N	-4.0206990	1.2708270	0.0512460
C	3.2211030	1.8287670	0.0018200	C	-4.1392170	-0.0752300	0.0234000
C	1.8681940	1.3173120	-0.0540610	H	-5.7171510	-2.8792050	0.0384710
O	0.8472720	2.0249480	-0.0867330	H	-1.5177700	3.2864650	0.1617230
N	1.7223920	-0.0581500	-0.0733250	H	-3.2055020	3.6279330	0.2012240
				H	-0.7541710	1.2169410	-0.1032820
				C	-6.6425440	-0.2093540	0.1513700

H -6.7731690 0.2910670 1.1123460
H -6.7916840 0.5074160 -0.6571390
H -7.3662960 -1.0180570 0.0594490