Supporting Information

Theoretical Studies on the Thermodynamics and Kinetics of the Glycosidic Bond Cleavage in Deoxythymidine Glycol

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THE GASE PHASE STRUCTURES

DIRECT CLEAVAGE PATHWAY

1A-RC (E= -1026.53896902)

Sum of electronic and zero-point Energies= -1026.245743
Sum of electronic and thermal Energies= -1026.227705
Sum of electronic and thermal Enthalpies= -1026.226761
Sum of electronic and thermal Free Energies= -1026.292860

H	-1.642071	2.280090	-1.039799
O	-2.441641	2.375633	-0.533678
C	-3.349052	1.400318	-0.984432
H	-3.506817	1.487968	-2.057798
H	-4.294726	1.586759	-0.488350
C	-2.895905	-0.001947	-0.653800
H	-3.591287	-0.712839	-1.103421
O	-1.589818	-0.192087	-1.166427
C	-0.928019	-1.220680	-0.452801
H	-0.865264	-2.108282	-1.063966
N	0.443561	-0.805634	-0.230586
C	0.709109	0.349332	0.580141
H	-0.131038	1.026590	0.468472
C	1.975901	1.059993	0.105848
C	1.789152	1.723398	-1.253268
H	1.054773	2.515670	-1.154720
H	2.724367	2.168463	-1.574787
H	1.453911	1.021045	-2.007606
C	3.104212	0.045823	0.032188
O	4.235502	0.349542	0.296286
N	2.738156	-1.193828	-0.384701
H	3.461222	-1.873905	-0.531969
C	1.441097	-1.664448	-0.590644
O	1.275909	-2.753700	-1.065808
C	-2.775995	-0.330437	0.824482
H	-2.390718	0.537435	1.354397
C	-1.762208	-1.469351	0.814910
H	-1.144088	-1.513807	1.700843
H	-2.300705	-2.405989	0.715722
O	-4.047464	-0.676528	1.313040
H	-4.042157	-0.668338	2.263022
O	2.299537	2.012432	1.081156
H	3.254382	2.052308	1.143185
O	0.845148	-0.045525	1.919432

H	1.221055	0.692936	2.396039

1A-TS (E= -1026.46027477)

Sum of electronic and zero-point Energies=	-1026.171349
Sum of electronic and thermal Energies=	-1026.153665
Sum of electronic and thermal Enthalpies=	-1026.152721
Sum of electronic and thermal Free Energies=	-1026.217284

H	-0.858709	-0.841138	1.140641
O	-1.551289	-1.538485	1.246288
C	-2.761507	-1.025848	1.670994
H	-2.683339	-0.463769	2.602132
H	-3.436285	-1.859749	1.850178
C	-3.428361	-0.140364	0.636752
H	-4.464800	0.055571	0.873778
O	-2.774440	1.191742	0.693793
C	-2.073009	1.408896	-0.311038
H	-1.500460	2.323096	-0.317189
N	0.474318	0.051102	0.506580
C	1.270632	-0.927497	-0.154348
H	0.992125	-1.911133	0.218352
C	2.775428	-0.751950	0.053370
C	3.179876	-1.092431	1.482776
H	2.968020	-2.140425	1.666318
H	4.244122	-0.927882	1.614616
H	2.635526	-0.493661	2.203940
C	3.150063	0.686889	-0.246283
O	4.216495	0.966384	-0.738331
N	2.218189	1.593345	0.112719
H	2.434440	2.565951	0.002256
C	0.887648	1.297946	0.501874
O	0.198379	2.281226	0.790303
C	-3.253369	-0.561623	-0.818405
H	-2.961437	-1.602576	-0.870530
C	-2.136680	0.358955	-1.333214
H	-1.153209	-0.112728	-1.385964
H	-2.351302	0.788477	-2.308061
O	-4.478497	-0.327160	-1.470231
H	-4.495191	-0.780266	-2.306342
O	3.448138	-1.585934	-0.858492
H	4.232971	-1.115743	-1.141475
O	0.973609	-0.875663	-1.547815
H	1.626509	-1.409861	-1.996725

1A-PC (E= -1026.50782478)

Sum of electronic and zero-point Energies= -1026.214539
Sum of electronic and thermal Energies= -1026.197067
Sum of electronic and thermal Enthalpies= -1026.196123
Sum of electronic and thermal Free Energies= -1026.259711

H	-0.975354	1.585995	0.149598
O	-1.709540	2.203062	0.250401
C	-2.659962	1.953186	-0.742667
H	-2.275910	2.188855	-1.735492
H	-3.506727	2.606533	-0.551434
C	-3.142509	0.520074	-0.750073
H	-3.984836	0.419590	-1.427663
O	-2.088107	-0.326557	-1.219815
C	-1.828178	-1.341532	-0.314953
H	-2.307403	-2.262253	-0.627889
N	0.453514	0.334552	0.208389
C	1.668689	0.992673	0.627100
H	1.533362	2.062510	0.489410
C	2.890018	0.546450	-0.182652
C	2.822750	1.028660	-1.627784
H	2.827644	2.113143	-1.632281
H	3.692198	0.678977	-2.173942
H	1.927208	0.682795	-2.132232
C	2.953281	-0.970476	-0.158475
O	3.991172	-1.570734	-0.130461
N	1.736009	-1.582061	-0.219557
H	1.700428	-2.580804	-0.300772
C	0.547390	-0.882990	-0.101620
O	-0.453040	-1.704758	-0.374822
C	-3.544091	-0.024960	0.622969
H	-3.735395	0.780853	1.323016
C	-2.343237	-0.867082	1.033481
H	-1.602952	-0.251714	1.526377
H	-2.614498	-1.692844	1.680989
O	-4.705811	-0.810884	0.434311
H	-5.026139	-1.109647	1.278248
O	4.029741	1.055569	0.454982
H	4.729011	0.407707	0.373358
O	1.859657	0.696606	1.982422
H	2.715230	1.040425	2.230786

2A-RC (E= -1105.10356496)

Sum of electronic and zero-point Energies= -1104.753037

Sum of electronic and thermal Energies= -1104.732131
Sum of electronic and thermal Enthalpies= -1104.731187
Sum of electronic and thermal Free Energies= -1104.804247

O	4.027770	-1.781276	-0.179623
C	2.649710	-1.635756	-0.351458
H	2.119289	-1.878397	0.573978
H	2.280043	-2.303793	-1.130635
C	2.365584	-0.205973	-0.757460
H	2.956712	0.048989	-1.630126
O	0.981835	-0.110011	-1.071485
C	0.395281	0.959244	-0.359086
H	0.421880	1.865217	-0.948609
N	-1.002398	0.646998	-0.151430
C	-1.359430	-0.572938	0.514418
H	-0.572724	-1.290144	0.309703
C	-2.674097	-1.117256	-0.039995
C	-2.530428	-1.613335	-1.473522
H	-1.827219	-2.438410	-1.489736
H	-3.489483	-1.969803	-1.833259
H	-2.168836	-0.837322	-2.137930
C	-3.720080	-0.017887	0.021616
O	-4.873205	-0.263427	0.251720
N	-3.256565	1.232293	-0.236101
H	-3.923096	1.980292	-0.290682
C	-1.925006	1.620113	-0.395414
O	-1.671260	2.742608	-0.734773
C	2.641516	0.820080	0.343384
H	3.322957	0.417911	1.089383
C	1.248775	1.101925	0.891808
H	0.962357	0.359773	1.629593
H	1.153991	2.081023	1.343828
O	3.213648	1.952852	-0.261113
O	-3.075643	-2.158477	0.809085
H	-4.031289	-2.133650	0.865658
O	-1.469748	-0.336552	1.893047
H	-1.918321	-1.089551	2.274249
C	3.812762	2.850985	0.631031
H	4.247750	3.646084	0.039415
H	3.092719	3.286099	1.322958
H	4.600632	2.363363	1.205460
C	4.416084	-3.081758	0.160085
H	4.135809	-3.793684	-0.616629
H	5.493147	-3.082519	0.266909

H	3.965223	-3.396914	1.101882

2A-TS (E= -1105.01677300)

Sum of electronic and zero-point Energies=	-1104.670170
Sum of electronic and thermal Energies=	-1104.649046
Sum of electronic and thermal Enthalpies=	-1104.648102
Sum of electronic and thermal Free Energies=	-1104.721919

O	-2.780232	2.134551	-0.481443
C	-2.187525	1.178433	-1.306655
H	-1.102031	1.202091	-1.252877
H	-2.488734	1.315721	-2.346561
C	-2.679251	-0.164654	-0.820136
H	-3.748937	-0.262452	-0.950921
O	-2.070110	-1.173155	-1.699513
C	-1.406208	-2.015451	-1.053874
H	-0.899436	-2.782423	-1.608838
N	0.696873	-0.309302	-0.561736
C	1.172264	0.629404	0.392086
H	0.628756	1.567692	0.265721
C	2.664489	0.952679	0.268320
C	2.949239	1.780092	-0.979662
H	2.441089	2.734932	-0.890659
H	4.014572	1.966811	-1.064925
H	2.603665	1.279300	-1.876776
C	3.449542	-0.343582	0.197963
O	4.549067	-0.433639	0.689878
N	2.832004	-1.330021	-0.479359
H	3.324316	-2.190938	-0.625293
C	1.470123	-1.315524	-0.880177
O	1.106448	-2.316778	-1.511269
C	-2.287015	-0.583627	0.597487
H	-1.619552	0.143668	1.044435
C	-1.550443	-1.919629	0.402448
H	-0.596460	-1.994733	0.902799
H	-2.183941	-2.755136	0.711024
O	-3.461605	-0.711577	1.342608
O	3.066278	1.654015	1.419953
H	3.950102	1.352947	1.634807
O	0.898802	0.137267	1.699546
H	1.402965	0.672363	2.310397
C	-3.261007	-0.707911	2.734293
H	-4.238432	-0.767262	3.193961
H	-2.664541	-1.560197	3.057528

H	-2.766640	0.207242	3.052894
C	-2.390765	3.447477	-0.783217
H	-2.672841	3.717205	-1.800790
H	-2.901074	4.101939	-0.089149
H	-1.314821	3.574768	-0.670442

2A-PC (E= -1105.06587558)

Sum of electronic and zero-point Energies=	-1104.715938
Sum of electronic and thermal Energies=	-1104.695007
Sum of electronic and thermal Enthalpies=	-1104.694063
Sum of electronic and thermal Free Energies=	-1104.766863

O	-3.118850	2.098723	-0.318737
C	-2.161603	1.391489	-1.052381
H	-1.159953	1.566188	-0.661985
H	-2.179455	1.692620	-2.101445
C	-2.482497	-0.082760	-0.958966
H	-3.487699	-0.257955	-1.331769
O	-1.554199	-0.775824	-1.787723
C	-1.028281	-1.895483	-1.179258
H	-1.227036	-2.765890	-1.790391
N	0.657964	-0.096966	0.197766
C	1.599183	0.639667	0.999356
H	1.160371	1.608174	1.230588
C	2.935006	0.877386	0.284408
C	2.789025	1.863449	-0.869968
H	2.481748	2.823486	-0.469419
H	3.742658	1.990931	-1.370855
H	2.051784	1.534857	-1.594311
C	3.446349	-0.448428	-0.252257
O	4.615498	-0.718595	-0.281559
N	2.472099	-1.266712	-0.736182
H	2.736503	-2.121393	-1.188850
C	1.124791	-1.006572	-0.532863
O	0.406812	-1.868612	-1.232018
C	-2.385548	-0.693937	0.438219
H	-1.829568	-0.039534	1.101136
C	-1.631009	-2.009377	0.214674
H	-0.877625	-2.209087	0.963690
H	-2.349022	-2.823084	0.217595
O	-3.684028	-0.886183	0.928598
O	3.847684	1.361638	1.232349
H	4.706708	0.992272	1.028519
O	1.810236	-0.086272	2.179928

H	2.532509	0.332365	2.643949
C	-3.747925	-1.097250	2.310614
H	-4.794122	-1.188753	2.573361
H	-3.230544	-2.010174	2.607433
H	-3.316422	-0.258627	2.856511
C	-2.925213	3.481711	-0.346597
H	-2.977385	3.869679	-1.364896
H	-3.712881	3.934025	0.242588
H	-1.959893	3.757269	0.080876

ABSTRACTION CLEAVAGE PATHWAY

1B-RC (E= -1026.53024780)

Sum of electronic and zero-point Energies=	-1026.236476
Sum of electronic and thermal Energies=	-1026.218870
Sum of electronic and thermal Enthalpies=	-1026.217926
Sum of electronic and thermal Free Energies=	-1026.281881

H	2.200220	2.148021	0.197867
O	3.156168	2.106630	0.251813
C	3.533052	1.110943	1.159771
H	3.190095	1.339724	2.168577
H	4.619139	1.090692	1.173856
C	3.021669	-0.263450	0.784440
H	3.484654	-1.011360	1.422498
O	1.610614	-0.302378	0.982969
C	0.958889	-0.738018	-0.181551
H	0.806905	-1.807107	-0.129825
N	-0.378175	-0.161600	-0.228478
C	-1.515929	-1.092399	-0.274377
C	-2.824856	-0.441555	0.188359
C	-2.990744	0.977145	-0.338265
O	-4.063008	1.495832	-0.472801
N	-1.824215	1.643547	-0.550419
H	-1.882222	2.630305	-0.725589
C	-0.525206	1.174524	-0.373862
O	0.374552	1.978860	-0.400576
C	3.263254	-0.648117	-0.677673
H	4.041962	-0.036278	-1.120306
C	1.908070	-0.414097	-1.330757
H	1.818382	0.618078	-1.637666
H	1.746961	-1.062713	-2.185670
O	3.634626	-2.014901	-0.694203

H	3.853875	-2.270727	-1.583208
C	-4.010105	-1.303134	-0.192040
H	-3.884837	-2.296663	0.220126
H	-4.924854	-0.859757	0.183559
H	-4.103690	-1.375935	-1.270668
O	-2.690652	-0.323601	1.594392
H	-3.525605	-0.074164	1.978925
O	-1.264765	-2.211115	0.495022
H	-1.350320	-1.961034	1.414982
H	-1.642774	-1.450372	-1.292376

1B-TS (E= -1026.44579296)

Sum of electronic and zero-point Energies=	-1026.161191
Sum of electronic and thermal Energies=	-1026.142832
Sum of electronic and thermal Enthalpies=	-1026.141888
Sum of electronic and thermal Free Energies=	-1026.208558

H	-1.503756	-1.759084	0.766262
O	-2.290701	-1.891183	1.303719
C	-2.763169	-0.702160	1.853663
H	-2.013176	-0.201728	2.464119
H	-3.582875	-0.981953	2.506478
C	-3.309171	0.316808	0.850780
H	-4.166494	0.832328	1.260236
O	-2.320426	1.387733	0.624401
C	-1.898354	1.343790	-0.578663
H	-1.196553	2.102815	-0.864964
N	0.659688	0.508257	-0.370863
C	1.931981	1.171822	-0.400706
C	3.074578	0.329929	0.184379
C	3.022418	-1.097521	-0.368225
O	3.980828	-1.821744	-0.385108
N	1.786453	-1.507480	-0.769020
H	1.665965	-2.478681	-0.988281
C	0.626891	-0.745814	-0.604756
O	-0.461868	-1.418679	-0.719902
C	-3.613582	-0.203903	-0.551014
H	-3.716221	-1.281476	-0.539857
C	-2.390043	0.267117	-1.325695
H	-1.433423	-0.559737	-1.077448
H	-2.430232	0.353698	-2.400323
O	-4.809771	0.411516	-0.981701
H	-5.112297	-0.001447	-1.783030
C	4.427231	0.957356	-0.072477

H	4.446869	1.951950	0.355692
H	5.212684	0.350056	0.363837
H	4.623844	1.029017	-1.137587
O	2.806514	0.229098	1.574319
H	3.548478	-0.181398	2.007418
O	1.847045	2.399045	0.256325
H	1.669135	2.213330	1.175424
H	2.199424	1.416032	-1.428939

1B-PC (E= -1026.48242394)

Sum of electronic and zero-point Energies=	-1026.193833
Sum of electronic and thermal Energies=	-1026.173939
Sum of electronic and thermal Enthalpies=	-1026.172995
Sum of electronic and thermal Free Energies=	-1026.246213

H	-2.320077	-1.288271	1.806100
O	-3.101304	-1.721604	1.477973
C	-4.185436	-0.835768	1.593304
H	-4.279897	-0.463579	2.611732
H	-5.081898	-1.399295	1.356655
C	-4.073098	0.329276	0.641333
H	-4.921294	0.995777	0.761084
O	-2.881620	1.066487	0.971808
C	-2.156781	1.207670	-0.154030
H	-1.243812	1.763167	-0.050797
N	1.129145	0.553325	-0.461359
C	2.421064	1.189390	-0.379527
C	3.502989	0.296950	0.249689
C	3.447243	-1.120778	-0.327492
O	4.385934	-1.864780	-0.338177
N	2.206038	-1.509883	-0.753559
H	2.069003	-2.475930	-0.985600
C	1.103218	-0.683580	-0.669357
O	-0.015011	-1.374189	-0.847110
C	-3.955940	-0.046807	-0.843800
H	-3.929439	-1.127090	-0.971947
C	-2.658395	0.603520	-1.222095
H	-0.765173	-0.770425	-0.827849
H	-2.236391	0.624297	-2.208767
O	-5.094169	0.475994	-1.504847
H	-5.100364	0.182620	-2.409193
C	4.884516	0.890733	0.090095
H	4.903723	1.875926	0.539113
H	5.625584	0.253995	0.560777

H	5.148219	0.977553	-0.959084
O	3.140890	0.171075	1.615900
H	3.860917	-0.220804	2.100378
O	2.328238	2.390148	0.309960
H	2.100672	2.186856	1.214188
H	2.743996	1.452426	-1.385145

2B-RC (E= -1105.08764228)

Sum of electronic and zero-point Energies=	-1104.737179
Sum of electronic and thermal Energies=	-1104.716215
Sum of electronic and thermal Enthalpies=	-1104.715271
Sum of electronic and thermal Free Energies=	-1104.788380

O	-0.995878	2.052961	0.128894
C	-1.841494	1.908186	-0.973706
H	-1.364922	2.300044	-1.873847
H	-2.774580	2.455795	-0.818616
C	-2.162846	0.450549	-1.187803
H	-2.914587	0.379161	-1.970001
O	-1.003881	-0.252394	-1.621318
C	-0.706500	-1.347535	-0.783001
H	-0.430165	-2.166305	-1.429349
N	0.492172	-1.055195	0.006991
C	1.771919	-1.184234	-0.715165
C	2.780516	-0.108388	-0.306473
C	2.837247	0.034137	1.208252
O	3.774847	0.520859	1.778338
N	1.722408	-0.386555	1.866340
H	1.681821	-0.192894	2.850504
C	0.478989	-0.729800	1.320548
O	-0.473129	-0.744569	2.056076
C	-2.686044	-0.284602	0.045905
H	-2.374744	0.220593	0.953507
C	-2.007108	-1.647084	-0.053881
H	-1.874349	-2.145736	0.892153
H	-2.600297	-2.271401	-0.717055
O	-4.086442	-0.326740	-0.028183
C	4.152629	-0.430122	-0.863111
H	4.095224	-0.501023	-1.942025
H	4.855791	0.344266	-0.578605
H	4.524340	-1.369405	-0.465864
O	2.284272	1.110230	-0.821043
H	2.949986	1.783695	-0.721536
O	1.569461	-1.163734	-2.078654

H	1.161874	-0.329491	-2.313576
H	2.205403	-2.156674	-0.492444
C	-4.708832	-0.735116	1.159443
H	-5.777752	-0.667305	1.000882
H	-4.455960	-1.763401	1.415047
H	-4.428713	-0.091460	1.992694
C	-0.490106	3.345491	0.281389
H	0.135849	3.349339	1.164751
H	0.110383	3.637842	-0.580658
H	-1.290893	4.074815	0.413473

2B-TS (E= -1105.00671051)

Sum of electronic and zero-point Energies=	-1104.665249
Sum of electronic and thermal Energies=	-1104.643692
Sum of electronic and thermal Enthalpies=	-1104.642748
Sum of electronic and thermal Free Energies=	-1104.717376

O	-0.990893	1.807739	-0.352015
C	-1.834297	1.603285	-1.435346
H	-1.275964	1.559360	-2.371887
H	-2.569852	2.408108	-1.521065
C	-2.578036	0.309496	-1.245254
H	-3.362911	0.218987	-1.984730
O	-1.673431	-0.810508	-1.497466
C	-1.545403	-1.525373	-0.443538
H	-0.973696	-2.424813	-0.548895
N	0.830271	-1.184095	0.408141
C	2.068012	-1.456917	-0.253502
C	3.041350	-0.268642	-0.306206
C	3.073248	0.479502	1.028605
O	3.983540	1.209480	1.328856
N	1.970995	0.321220	1.800849
H	1.887318	0.897795	2.617089
C	0.811813	-0.374569	1.405068
O	-0.208771	-0.123395	2.109014
C	-3.143793	0.048443	0.153603
H	-3.106896	0.947373	0.762078
C	-2.225501	-1.041353	0.688760
H	-1.282123	-0.573056	1.376869
H	-2.631881	-1.784124	1.360227
O	-4.479418	-0.361539	-0.011504
C	4.433185	-0.705719	-0.710244
H	4.387386	-1.207037	-1.669616
H	5.096191	0.150654	-0.769706

H	4.849263	-1.389228	0.023066
O	2.500575	0.646655	-1.253025
H	3.152204	1.317881	-1.430033
O	1.829971	-1.928924	-1.549548
H	1.524764	-1.186100	-2.065040
H	2.581597	-2.273762	0.253493
C	-5.224916	-0.394101	1.176508
H	-6.238239	-0.663328	0.909032
H	-4.840046	-1.131320	1.879003
H	-5.230352	0.581488	1.661927
C	-0.134860	2.908472	-0.491256
H	0.454008	2.971187	0.413521
H	0.533152	2.776004	-1.340131
H	-0.700191	3.832861	-0.615808

2B-PC (E= -1105.05369064)

Sum of electronic and zero-point Energies=	-1104.706741
Sum of electronic and thermal Energies=	-1104.684325
Sum of electronic and thermal Enthalpies=	-1104.683381
Sum of electronic and thermal Free Energies=	-1104.761707

O	-2.378064	-1.717317	-0.784155
C	-3.536176	-0.919167	-0.838729
H	-4.412117	-1.538948	-0.650073
H	-3.632991	-0.477508	-1.831642
C	-3.485378	0.189961	0.175108
H	-4.369349	0.806486	0.044970
O	-3.523238	-0.362592	1.494623
C	-2.487563	0.166484	2.183260
H	-2.410459	-0.163827	3.201853
N	0.894651	-0.242401	-0.691230
C	2.092560	0.429066	-1.125359
C	3.223679	0.413085	-0.084338
C	3.371101	-0.973336	0.548012
O	4.384850	-1.352305	1.064686
N	2.226461	-1.717243	0.555923
H	2.218115	-2.559792	1.099602
C	1.024871	-1.246242	0.051705
O	0.025648	-2.008980	0.452009
C	-2.254989	1.110068	0.105938
H	-1.527378	0.776392	-0.631795
C	-1.716547	0.994435	1.502413
H	-0.815167	-1.703623	0.073560
H	-0.830409	1.468806	1.873153

O	-2.711893	2.395822	-0.258124
C	4.537010	0.878288	-0.673304
H	4.413797	1.873679	-1.081730
H	5.311197	0.882133	0.086168
H	4.861285	0.211380	-1.465828
O	2.788030	1.270461	0.960860
H	3.510840	1.430406	1.559796
O	1.810624	1.738831	-1.497303
H	1.583273	2.216988	-0.703542
H	2.459105	-0.057994	-2.027240
C	-1.684878	3.304946	-0.544479
H	-2.153081	4.217649	-0.891105
H	-1.092544	3.533464	0.341403
H	-1.024080	2.923413	-1.322405
C	-2.402218	-2.785691	-1.698625
H	-1.481724	-3.341340	-1.576695
H	-3.245904	-3.444053	-1.500152
H	-2.466692	-2.418959	-2.721537

S_N1 PATHWAY

1C-RC (E= -1102.95480249)

Sum of electronic and zero-point Energies=	-1102.635819
Sum of electronic and thermal Energies=	-1102.614748
Sum of electronic and thermal Enthalpies=	-1102.613804
Sum of electronic and thermal Free Energies=	-1102.686355

H	-1.802464	-2.590196	0.076226
O	-2.753830	-2.671771	0.163867
C	-3.216431	-1.796119	1.151636
H	-2.822079	-2.054809	2.133897
H	-4.297123	-1.902468	1.186987
C	-2.871361	-0.348787	0.867479
H	-3.415222	0.296436	1.553210
O	-1.476041	-0.162532	1.065917
C	-0.880479	0.435891	-0.059913
H	-0.825855	1.505937	0.081888
N	0.501895	-0.006103	-0.166143
C	1.532040	1.033261	-0.032828
C	2.924405	0.453366	0.248700
C	3.204240	-0.824754	-0.530049
O	4.311983	-1.177529	-0.821844
N	2.106246	-1.593287	-0.762478

H	2.256076	-2.531209	-1.086736
C	0.777990	-1.290953	-0.480933
O	-0.038846	-2.175314	-0.582339
C	-3.175263	0.085520	-0.569818
H	-3.839299	-0.620610	-1.053076
C	-1.805698	0.126223	-1.234754
H	-1.584235	-0.839540	-1.665851
H	-1.747270	0.891685	-2.000029
O	-3.799652	1.367662	-0.524333
H	-4.233917	1.530436	-1.355125
C	3.992739	1.494674	-0.003740
H	3.784517	2.378119	0.587134
H	4.967130	1.097392	0.255789
H	4.022551	1.768783	-1.053081
O	2.883125	0.061880	1.612028
H	3.761537	-0.148234	1.914213
O	1.196423	1.923310	0.968990
H	1.352832	1.492083	1.808616
H	1.568075	1.614490	-0.949143
H	-2.706313	2.942431	-0.388241
O	-2.021749	3.577632	-0.605483
H	-2.000312	4.208381	0.104559

1C-TS1 (E= -1102.87167035)

Sum of electronic and zero-point Energies=	-1102.561840
Sum of electronic and thermal Energies=	-1102.540187
Sum of electronic and thermal Enthalpies=	-1102.539243
Sum of electronic and thermal Free Energies=	-1102.613650

H	-0.989490	-2.215246	0.402144
O	-1.733707	-2.580256	0.891420
C	-2.330682	-1.640758	1.728688
H	-1.630630	-1.227128	2.452840
H	-3.094195	-2.178070	2.281040
C	-3.017070	-0.470878	1.020393
H	-3.910494	-0.179762	1.555800
O	-2.163288	0.723329	1.061837
C	-1.817139	1.054578	-0.122814
H	-1.227133	1.943262	-0.220483
N	0.889765	0.510804	-0.205936
C	2.095610	1.283804	-0.111439
C	3.338529	0.444891	0.219772
C	3.384444	-0.812420	-0.652827
O	4.401230	-1.415169	-0.869725

N	2.170418	-1.237531	-1.099824
H	2.124364	-2.137475	-1.539765
C	0.958363	-0.650140	-0.726748
O	-0.069813	-1.386871	-0.967685
C	-3.312965	-0.667163	-0.464866
H	-3.284885	-1.717651	-0.720654
C	-2.200941	0.141052	-1.109715
H	-1.127693	-0.596620	-1.082184
H	-2.305393	0.487016	-2.125252
O	-4.609340	-0.139146	-0.737428
H	-4.953144	-0.535649	-1.530659
C	4.614039	1.246103	0.076786
H	4.567778	2.110965	0.727045
H	5.473174	0.635387	0.332020
H	4.745588	1.582607	-0.946838
O	3.157002	-0.005245	1.553726
H	3.955179	-0.430546	1.851273
O	1.939490	2.305265	0.824631
H	1.814548	1.889829	1.674540
H	2.285071	1.789771	-1.058137
H	-4.541081	1.826459	-0.690642
O	-4.045089	2.645041	-0.647981
H	-4.607856	3.289950	-0.235515

1C-IM (E= -1102.90979927)

Sum of electronic and zero-point Energies=	-1102.595605
Sum of electronic and thermal Energies=	-1102.572488
Sum of electronic and thermal Enthalpies=	-1102.571543
Sum of electronic and thermal Free Energies=	-1102.653441

H	1.949090	1.484814	1.730121
O	2.700686	1.811955	1.247871
C	3.794116	0.955077	1.476330
H	3.914854	0.751098	2.538165
H	4.686279	1.457574	1.122524
C	3.655618	-0.347652	0.726336
H	4.511924	-0.978722	0.938924
O	2.476080	-1.031326	1.201656
C	1.666132	-1.238635	0.151119
H	0.732772	-1.723103	0.367847
N	-1.553841	-0.522945	-0.354890
C	-2.842672	-1.170527	-0.339650
C	-3.973181	-0.274352	0.191634
C	-3.889504	1.131691	-0.410012

O	-4.831435	1.866449	-0.497197
N	-2.626453	1.523101	-0.762443
H	-2.482398	2.484257	-1.010322
C	-1.524876	0.708976	-0.591197
O	-0.403981	1.406467	-0.716630
C	3.475706	-0.194213	-0.799057
H	3.547867	0.845110	-1.095605
C	2.118108	-0.781005	-1.010859
H	0.348294	0.809749	-0.657176
H	1.620881	-0.865283	-1.957592
O	4.498165	-0.849255	-1.543188
H	4.338316	-1.788515	-1.531992
C	-5.335471	-0.884364	-0.051586
H	-5.377350	-1.862135	0.411947
H	-6.112399	-0.247121	0.356355
H	-5.525975	-0.990954	-1.114691
O	-3.708754	-0.117398	1.577021
H	-4.460891	0.284550	2.000709
O	-2.784465	-2.349968	0.389947
H	-2.646508	-2.115864	1.304882
H	-3.095198	-1.465801	-1.356319
H	6.134303	-0.093826	-0.894221
O	6.663394	0.374956	-0.245875
H	7.436820	0.688057	-0.699419

1C-TS2 (E= -1102.82582073)

Sum of electronic and zero-point Energies=	-1102.513174
Sum of electronic and thermal Energies=	-1102.492087
Sum of electronic and thermal Enthalpies=	-1102.491142
Sum of electronic and thermal Free Energies=	-1102.565608

H	1.430542	2.549317	-0.189026
O	2.383169	2.521651	-0.178254
C	2.816692	1.780946	0.933240
H	2.233760	2.022014	1.820422
H	3.847261	2.055790	1.131935
C	2.787549	0.297791	0.678605
H	3.029646	-0.284470	1.557589
O	1.383275	-0.064363	0.376077
C	1.323827	-0.762334	-0.663678
H	0.338002	-1.115218	-0.926408
N	-2.036438	0.936093	-1.405425
C	-3.085338	0.005772	-1.045290
C	-2.790946	-0.726285	0.272685

C	-2.376516	0.278947	1.355027
O	-2.527031	0.096637	2.525532
N	-1.741520	1.400478	0.871669
H	-1.330786	2.028717	1.536772
C	-1.504986	1.574959	-0.470031
O	-0.602488	2.542105	-0.687690
C	3.607592	-0.227978	-0.519211
H	3.999778	0.603634	-1.093223
C	2.562387	-1.015292	-1.333949
H	-0.587663	2.709462	-1.630266
H	2.529638	-0.899156	-2.409848
O	4.661269	-1.006965	-0.090337
H	4.217086	-1.813287	0.298512
C	-3.962023	-1.561338	0.736118
H	-4.209517	-2.287231	-0.027920
H	-3.720186	-2.066893	1.664442
H	-4.829932	-0.936797	0.920646
O	-1.646007	-1.526808	0.011200
H	-1.510461	-2.146237	0.723781
O	-3.320862	-0.892246	-2.070772
H	-2.536025	-1.418526	-2.197589
H	-4.012613	0.562004	-0.922223
H	2.709122	-2.095370	-1.040710
O	2.872293	-2.693414	0.587871
H	2.949679	-3.507663	1.069295

1C-PC (E= -1102.94537051)

Sum of electronic and zero-point Energies=	-1102.625069
Sum of electronic and thermal Energies=	-1102.604783
Sum of electronic and thermal Enthalpies=	-1102.603839
Sum of electronic and thermal Free Energies=	-1102.675820

H	-2.990443	2.024091	1.568567
O	-3.672050	2.222318	0.934872
C	-3.143860	2.013814	-0.350739
H	-2.240715	2.604276	-0.498279
H	-3.889763	2.359173	-1.058581
C	-2.838787	0.558211	-0.621246
H	-2.434428	0.457111	-1.624785
O	-1.852210	0.130654	0.334765
C	-2.219438	-1.131874	0.869573
H	-1.753696	-1.196847	1.847281
N	2.903273	1.693318	-0.378993
C	3.643832	0.493406	-0.680445

C	3.134326	-0.739081	0.084564
C	1.605408	-0.807015	0.040240
O	1.001945	-1.846566	0.167502
N	0.972887	0.388485	-0.059240
H	-0.037392	0.412455	0.063207
C	1.680661	1.570259	-0.140219
O	0.880948	2.616383	0.063934
C	-4.024232	-0.411558	-0.462377
H	-4.963668	0.124499	-0.449186
C	-3.730376	-1.093987	0.869931
H	1.414091	3.403630	-0.034834
H	-4.081152	-0.479507	1.690993
O	-4.106542	-1.321477	-1.530554
H	-3.365311	-1.921032	-1.469225
C	3.752773	-2.016381	-0.436727
H	4.830971	-1.942027	-0.368943
H	3.402791	-2.868318	0.136022
H	3.477350	-2.184421	-1.472905
O	3.463560	-0.511445	1.444944
H	3.381447	-1.325537	1.931703
O	4.997257	0.680472	-0.450019
H	5.110063	0.883766	0.475194
H	3.552445	0.288506	-1.745719
H	-4.173122	-2.079066	0.935245
O	-1.799980	-2.164741	0.043043
H	-0.837865	-2.192923	0.038654

2C-RC (E= -1181.51152785)

Sum of electronic and zero-point Energies=	-1181.135489
Sum of electronic and thermal Energies=	-1181.111286
Sum of electronic and thermal Enthalpies=	-1181.110342
Sum of electronic and thermal Free Energies=	-1181.191615

O	-2.704268	2.335178	-0.526324
C	-2.878263	1.331809	-1.481888
H	-2.321892	1.563128	-2.391184
H	-3.935009	1.236416	-1.746479
C	-2.383566	0.012575	-0.940623
H	-2.733005	-0.780421	-1.596597
O	-0.963440	0.001714	-0.913944
C	-0.520168	-0.413209	0.367187
H	-0.518102	-1.495353	0.399025
N	0.861772	-0.032914	0.531263
C	1.834300	-1.007523	0.009664

C	3.131687	-0.340063	-0.450253
C	3.618869	0.687905	0.562330
O	4.769971	1.012066	0.655088
N	2.634362	1.269097	1.299660
H	2.892735	2.062275	1.857938
C	1.251810	1.087134	1.193685
O	0.530023	1.889007	1.719465
C	-2.832990	-0.299204	0.491454
H	-3.711994	0.270430	0.777573
C	-1.604148	0.068901	1.314169
H	-1.563188	1.136781	1.451312
H	-1.566335	-0.426525	2.276894
O	-3.125077	-1.684586	0.539978
C	4.199396	-1.376967	-0.726145
H	3.842621	-2.075033	-1.473001
H	5.103360	-0.891192	-1.074697
H	4.451678	-1.922748	0.177255
O	2.782225	0.379525	-1.617964
H	3.571567	0.694302	-2.047789
O	1.281054	-1.727979	-1.035439
H	1.110927	-1.121479	-1.757028
H	2.065654	-1.735615	0.782657
H	-1.918046	-3.054990	-0.435818
O	-1.284652	-3.679717	-0.786265
H	-0.499764	-3.176571	-0.986636
C	-3.825291	-2.101709	1.683865
H	-4.779217	-1.581864	1.762787
H	-4.007238	-3.163234	1.578066
H	-3.255568	-1.932234	2.595208
C	-2.970798	3.622141	-1.003987
H	-2.801153	4.312683	-0.188147
H	-2.308384	3.880004	-1.830267
H	-4.004290	3.715560	-1.341037

2C-TS1 (E= -1181.43146147)

Sum of electronic and zero-point Energies=	-1181.064772
Sum of electronic and thermal Energies=	-1181.039823
Sum of electronic and thermal Enthalpies=	-1181.038879
Sum of electronic and thermal Free Energies=	-1181.121406

O	0.666366	-1.907498	-0.842076
C	1.579856	-1.491603	-1.800534
H	1.078888	-1.135240	-2.701837
H	2.249347	-2.306928	-2.089162

C	2.411818	-0.373169	-1.231914
H	3.251141	-0.167013	-1.883756
O	1.621821	0.851265	-1.211922
C	1.499577	1.282207	-0.014915
H	1.013206	2.228228	0.104334
N	-1.008815	0.918298	0.601364
C	-2.200432	1.500930	0.067776
C	-3.320842	0.492014	-0.228076
C	-3.465967	-0.512663	0.917365
O	-4.470390	-1.158347	1.079432
N	-2.356146	-0.673377	1.678344
H	-2.354991	-1.420420	2.347279
C	-1.107912	-0.080259	1.401544
O	-0.136818	-0.622030	2.007282
C	2.888804	-0.556902	0.212218
H	2.734409	-1.577352	0.545877
C	2.036978	0.442157	0.976958
H	1.001262	-0.094230	1.460527
H	2.461971	0.933735	1.839716
O	4.276953	-0.263803	0.249074
C	-4.637722	1.183934	-0.506782
H	-4.514558	1.865958	-1.339386
H	-5.407522	0.454279	-0.733982
H	-4.967752	1.745974	0.361167
O	-2.892274	-0.261409	-1.357262
H	-3.623064	-0.790524	-1.661286
O	-1.906377	2.234410	-1.086769
H	-1.638677	1.607262	-1.753853
H	-2.602549	2.232336	0.769410
H	4.469459	1.636949	-0.094510
O	4.132662	2.531884	-0.163410
H	4.748139	3.020503	-0.697145
C	4.923747	-0.713373	1.416832
H	4.813235	-1.790261	1.526744
H	5.973739	-0.472394	1.314562
H	4.532620	-0.224487	2.306172
C	-0.317179	-2.783270	-1.322639
H	-0.941358	-3.051899	-0.481559
H	-0.932158	-2.298700	-2.078360
H	0.130040	-3.686018	-1.740710

2C-IM (E= -1181.47831280)

Sum of electronic and zero-point Energies= -1181.106012

Sum of electronic and thermal Energies= -1181.080372

Sum of electronic and thermal Enthalpies= -1181.079428

Sum of electronic and thermal Free Energies= -1181.165468

O	1.791429	1.823968	-0.202577
C	2.622712	1.399217	0.856387
H	2.207871	1.733734	1.806771
H	3.620712	1.818413	0.746533
C	2.743018	-0.100169	0.856620
H	3.413911	-0.386052	1.660245
O	1.468098	-0.690574	1.117846
C	1.233925	-1.606907	0.157947
H	0.292126	-2.113011	0.237613
N	-1.630146	-0.253754	-0.190585
C	-2.730766	-1.171057	-0.312798
C	-4.075677	-0.596286	0.160690
C	-4.271128	0.835042	-0.348379
O	-5.350281	1.345264	-0.466124
N	-3.112507	1.520913	-0.574315
H	-3.177214	2.505817	-0.750192
C	-1.861094	0.966936	-0.354643
O	-0.933872	1.907507	-0.350395
C	3.257612	-0.724402	-0.452118
H	3.373235	0.020675	-1.239325
C	2.180924	-1.715115	-0.759745
H	-0.044689	1.536409	-0.233350
H	2.136738	-2.351215	-1.620534
O	4.546561	-1.276277	-0.194324
C	-5.236937	-1.476723	-0.244619
H	-5.086539	-2.472304	0.154393
H	-6.169699	-1.066150	0.126237
H	-5.314766	-1.538965	-1.325403
O	-3.967220	-0.492350	1.571692
H	-4.820338	-0.286315	1.940971
O	-2.449265	-2.351621	0.368591
H	-2.438932	-2.145347	1.300797
H	-2.836186	-1.455041	-1.358403
H	5.622431	0.054192	0.585810
O	5.938693	0.908069	0.893948
H	6.705906	0.737788	1.427211
C	5.135878	-1.893517	-1.310276
H	5.201162	-1.204045	-2.151813
H	6.135234	-2.195190	-1.022735
H	4.577249	-2.775135	-1.613366
C	1.930318	3.194486	-0.496345

H	1.244226	3.425950	-1.300252
H	1.682905	3.807526	0.368940
H	2.947373	3.417227	-0.811419

2C-TS2 (E= -1181.39041015)

Sum of electronic and zero-point Energies=	-1181.022477
Sum of electronic and thermal Energies=	-1180.998145
Sum of electronic and thermal Enthalpies=	-1180.997201
Sum of electronic and thermal Free Energies=	-1181.078839

O	-1.918543	2.258973	-0.599320
C	-3.004988	1.554916	-1.151603
H	-2.996722	1.653459	-2.236486
H	-3.940836	1.967921	-0.775670
C	-2.967970	0.103813	-0.779336
H	-3.855658	-0.385312	-1.166298
O	-1.837242	-0.537123	-1.407439
C	-1.406299	-1.476827	-0.639579
H	-0.571162	-2.048645	-0.988945
N	1.161731	-0.037408	-0.042748
C	2.144182	-1.079523	0.120962
C	3.596320	-0.597559	-0.026501
C	3.816778	0.725957	0.711397
O	4.892425	1.094054	1.089942
N	2.699466	1.505124	0.825106
H	2.815540	2.447793	1.146566
C	1.468318	1.122774	0.325099
O	0.638175	2.149443	0.295276
C	-2.844282	-0.253298	0.701252
H	-2.299080	0.518109	1.248342
C	-2.049567	-1.546329	0.626103
H	-0.228407	1.887591	-0.052787
H	-1.436724	-1.857016	1.457393
O	-4.143425	-0.338488	1.211964
C	4.584936	-1.644723	0.435801
H	4.427593	-2.558851	-0.123321
H	5.600804	-1.293353	0.292390
H	4.458555	-1.853722	1.493207
O	3.753665	-0.300472	-1.405189
H	4.676327	-0.167198	-1.599458
O	1.893906	-2.116409	-0.771727
H	2.129669	-1.806607	-1.644075
H	2.031795	-1.512131	1.113380
H	-2.734518	-2.491342	0.212180

O	-2.806756	-3.186243	-0.987933
H	-3.225755	-3.899837	-1.459060
C	-1.972440	3.642484	-0.861540
H	-1.101137	4.094619	-0.407058
H	-1.958578	3.834272	-1.932717
H	-2.871015	4.079678	-0.430921
C	-4.202558	-0.680021	2.569251
H	-5.244488	-0.653932	2.860614
H	-3.812099	-1.680641	2.743478
H	-3.644703	0.031269	3.180299

2C-PC (E= -1181.50262118)

Sum of electronic and zero-point Energies=	-1181.125927
Sum of electronic and thermal Energies=	-1181.102153
Sum of electronic and thermal Enthalpies=	-1181.101209
Sum of electronic and thermal Free Energies=	-1181.181840

O	2.137454	2.165962	-0.356307
C	3.288021	1.585187	0.211004
H	3.603941	2.167868	1.076229
H	4.098270	1.577526	-0.517619
C	3.007173	0.168651	0.626078
H	3.923506	-0.239545	1.054884
O	1.958884	0.145323	1.569010
C	1.429693	-1.159686	1.633713
H	0.361956	-1.042162	1.775607
N	-0.990618	0.119142	-0.454537
C	-2.043412	-0.724969	-0.959929
C	-3.376191	-0.579401	-0.207858
C	-3.702881	0.891743	0.058441
O	-4.816798	1.286362	0.264187
N	-2.614207	1.710468	0.127500
H	-2.753206	2.648657	0.453001
C	-1.313690	1.247309	-0.005210
O	-0.459940	2.164668	0.399662
C	2.532302	-0.771354	-0.471055
H	1.830446	-0.252743	-1.120332
C	1.804754	-1.854278	0.327749
H	0.461059	1.896714	0.237188
H	0.933732	-2.236835	-0.186147
O	3.640771	-1.206752	-1.206678
C	-4.513072	-1.258756	-0.938993
H	-4.272194	-2.304358	-1.085888
H	-5.433542	-1.166550	-0.373078

H	-4.678113	-0.797215	-1.907354
O	-3.152475	-1.164741	1.066980
H	-3.981193	-1.245327	1.529116
O	-1.646437	-2.058801	-0.954151
H	-1.646484	-2.351883	-0.045631
H	-2.217388	-0.475927	-2.005195
H	2.486541	-2.669006	0.547579
O	1.987929	-1.874933	2.696098
H	1.771249	-1.428496	3.508526
C	2.348370	3.466241	-0.844339
H	1.403775	3.826332	-1.230654
H	2.686508	4.131643	-0.051239
H	3.086289	3.463065	-1.644634
C	3.314099	-1.938520	-2.355979
H	4.241069	-2.166038	-2.867144
H	2.809782	-2.871543	-2.109082
H	2.671664	-1.361155	-3.021007

S_N2 PATHWAY

1D-RC (E= -1102.97074597)

Sum of electronic and zero-point Energies=	-1102.650797
Sum of electronic and thermal Energies=	-1102.630372
Sum of electronic and thermal Enthalpies=	-1102.629427
Sum of electronic and thermal Free Energies=	-1102.699033

H	-0.930164	-2.398259	-1.014979
O	-1.829264	-2.695294	-1.146729
C	-2.545813	-2.638081	0.058070
H	-2.096844	-3.282237	0.814289
H	-3.538833	-3.021972	-0.153935
C	-2.678692	-1.244218	0.633158
H	-3.335800	-1.273663	1.496326
O	-1.385166	-0.796652	1.076729
C	-1.044394	0.402145	0.446811
H	-1.281566	1.242425	1.087733
N	0.412818	0.418755	0.246364
C	1.137279	-0.821409	0.205263
H	0.743817	-1.447010	0.994819
C	2.628431	-0.592091	0.459535
C	2.897269	-0.276329	1.927674
H	2.605433	-1.131423	2.526742
H	3.956257	-0.096256	2.076214

H	2.342795	0.592670	2.264098
C	3.140343	0.552132	-0.394539
O	4.246711	0.545459	-0.857865
N	2.273757	1.591542	-0.530783
H	2.597875	2.425657	-0.985017
C	0.925758	1.587567	-0.193038
O	0.288624	2.611256	-0.302526
C	-3.170496	-0.168695	-0.338409
H	-3.761370	-0.600708	-1.139666
C	-1.869023	0.431099	-0.833440
H	-1.416947	-0.213442	-1.576720
H	-1.991119	1.421425	-1.246110
O	-3.942906	0.768339	0.377849
H	-3.639562	1.658904	0.202478
O	3.287848	-1.766170	0.075198
H	4.136191	-1.518665	-0.294084
O	0.926060	-1.445281	-1.037731
H	1.628159	-2.085383	-1.156206
O	-2.484133	3.365604	0.066371
H	-2.678078	4.265550	0.300389
H	-1.532424	3.299509	-0.042319

1D-TS (E= -1102.89153005)

Sum of electronic and zero-point Energies=	-1102.575276
Sum of electronic and thermal Energies=	-1102.555329
Sum of electronic and thermal Enthalpies=	-1102.554384
Sum of electronic and thermal Free Energies=	-1102.623300

H	1.047501	-2.397301	-0.079301
O	1.795633	-2.632006	0.473040
C	3.024825	-2.429203	-0.157987
H	3.049225	-2.862438	-1.156431
H	3.774928	-2.937238	0.439871
C	3.427618	-0.971375	-0.247566
H	4.432154	-0.860944	-0.631655
O	2.546919	-0.334439	-1.258332
C	1.667142	0.371739	-0.708681
H	0.872072	0.782097	-1.316228
N	-1.044061	0.597810	-1.122828
C	-1.708508	-0.641809	-0.958389
H	-1.853867	-1.095561	-1.935697
C	-3.075801	-0.540944	-0.275351
C	-4.110856	0.049828	-1.225933
H	-4.245369	-0.628785	-2.061456

H	-5.061843	0.161419	-0.715971
H	-3.795326	1.015080	-1.605438
C	-2.973476	0.343522	0.954922
O	-3.653128	0.130973	1.929623
N	-2.110515	1.373086	0.837908
H	-2.057144	2.039019	1.585682
C	-1.147336	1.509516	-0.194507
O	-0.425991	2.517866	-0.095335
C	3.182605	-0.103822	0.987075
H	3.298275	-0.685144	1.892059
C	1.749148	0.360443	0.764412
H	1.020846	-0.376443	1.096619
H	1.500395	1.311566	1.209381
O	4.076359	0.971865	1.035558
H	3.694039	1.738366	0.606395
O	-3.463683	-1.829071	0.137976
H	-3.947593	-1.727118	0.958508
O	-0.867883	-1.528085	-0.194356
H	-1.440174	-2.223837	0.131668
O	2.224535	2.817753	-0.574152
H	2.462787	3.459690	-1.234018
H	1.256875	2.885081	-0.449678

1D-PC (E= -1102.94872023)

Sum of electronic and zero-point Energies=	-1102.628041
Sum of electronic and thermal Energies=	-1102.608060
Sum of electronic and thermal Enthalpies=	-1102.607116
Sum of electronic and thermal Free Energies=	-1102.679606

H	-4.923254	-1.722170	-1.427951
O	-5.587692	-1.390464	-0.832603
C	-5.078328	-1.483547	0.473998
H	-4.794460	-2.508778	0.706709
H	-5.878536	-1.195740	1.147299
C	-3.888720	-0.577042	0.691245
H	-3.530376	-0.697902	1.710259
O	-2.863226	-0.978380	-0.225414
C	-2.287570	0.146877	-0.809363
H	-1.855584	-0.164143	-1.753818
N	1.367063	-0.075172	0.071901
C	2.327584	-1.147850	0.084556
H	1.978481	-1.904831	0.782484
C	3.720345	-0.684688	0.530567
C	3.750418	-0.323761	2.012182

H	3.521143	-1.212111	2.590397
H	4.741488	0.019097	2.289127
H	3.029371	0.447821	2.258641
C	4.119508	0.531383	-0.288460
O	5.250142	0.731932	-0.631502
N	3.093141	1.394004	-0.548923
H	3.294551	2.262855	-1.007991
C	1.778937	1.062494	-0.300057
O	0.983507	2.094320	-0.485790
C	-4.140557	0.919468	0.422766
H	-5.198244	1.131313	0.347316
C	-3.412573	1.153784	-0.898539
H	-4.056343	0.897890	-1.732339
H	-3.070989	2.175234	-1.006723
O	-3.655529	1.733147	1.463293
H	-2.706342	1.642482	1.494977
O	4.619621	-1.724771	0.259417
H	5.449940	-1.336148	-0.014485
O	2.391171	-1.674802	-1.211455
H	3.117496	-2.294635	-1.231372
O	-1.284103	0.683311	0.025663
H	-0.566640	0.041823	0.148335
H	0.061480	1.809056	-0.367953

2D-RC (E= -1181.53232597)

Sum of electronic and zero-point Energies=	-1181.156340
Sum of electronic and thermal Energies=	-1181.132033
Sum of electronic and thermal Enthalpies=	-1181.131089
Sum of electronic and thermal Free Energies=	-1181.211279

O	1.805494	-2.437358	-0.381994
C	2.685375	-1.672241	-1.159885
H	2.583473	-1.936538	-2.213359
H	3.718643	-1.855058	-0.859871
C	2.395384	-0.205335	-0.984409
H	3.142744	0.352747	-1.548115
O	1.101549	0.092217	-1.480387
C	0.504175	1.136392	-0.754594
H	0.317156	1.974481	-1.407413
N	-0.813280	0.673444	-0.306535
C	-0.926261	-0.592941	0.365556
H	-0.153310	-1.243799	-0.022723
C	-2.289028	-1.222014	0.086104
C	-2.427191	-1.658966	-1.367628

H	-1.676106	-2.412061	-1.576981
H	-3.408821	-2.092131	-1.526347
H	-2.289511	-0.832661	-2.055360
C	-3.371405	-0.214029	0.424052
O	-4.427593	-0.549700	0.885576
N	-3.062913	1.078576	0.129888
H	-3.772459	1.774993	0.264313
C	-1.825235	1.569029	-0.273633
O	-1.734521	2.736043	-0.579508
C	2.410759	0.308931	0.448180
H	2.008152	-0.445790	1.121006
C	1.477388	1.511474	0.365622
H	0.956982	1.731829	1.287316
H	2.036731	2.390479	0.063341
O	3.733532	0.599406	0.798927
O	-2.418175	-2.320278	0.948168
H	-3.335122	-2.371651	1.217995
O	-0.755514	-0.384773	1.745443
H	-0.983274	-1.201750	2.184739
O	0.513292	4.463968	-0.770641
H	0.318880	5.347238	-1.059899
H	-0.331452	4.016721	-0.691634
C	3.911261	0.930457	2.149420
H	3.393325	1.852418	2.408490
H	3.554334	0.132261	2.800451
H	4.973037	1.069013	2.308343
C	2.013877	-3.816521	-0.500414
H	3.015581	-4.094396	-0.171846
H	1.285945	-4.312517	0.128995
H	1.879317	-4.149576	-1.529802

2D-TS (E= -1181.45079939)

Sum of electronic and zero-point Energies=	-1181.078597
Sum of electronic and thermal Energies=	-1181.054634
Sum of electronic and thermal Enthalpies=	-1181.053690
Sum of electronic and thermal Free Energies=	-1181.134742

O	-2.305474	2.389957	-0.065668
C	-3.510889	1.915800	-0.572446
H	-3.670344	2.253159	-1.597468
H	-4.359012	2.249162	0.030093
C	-3.466458	0.412904	-0.538439
H	-4.403193	-0.020169	-0.859109
O	-2.465452	-0.019548	-1.525628

C	-1.463665	-0.542051	-0.977267
H	-0.621090	-0.812385	-1.584394
N	1.299123	-0.044236	-0.890613
C	1.911793	0.978392	-0.119376
H	1.759659	1.932284	-0.622804
C	3.419206	0.794914	0.082369
C	4.183315	1.041763	-1.212857
H	4.044678	2.076443	-1.508870
H	5.243037	0.867738	-1.057729
H	3.829627	0.398989	-2.010767
C	3.687063	-0.620486	0.559823
O	4.582403	-0.857609	1.336750
N	2.881099	-1.550217	0.015291
H	3.055694	-2.515967	0.218866
C	1.708727	-1.270676	-0.739478
O	1.149744	-2.282766	-1.202214
C	-2.996702	-0.211327	0.773417
H	-3.066063	0.503990	1.588707
C	-1.537937	-0.581224	0.485451
H	-0.818921	0.152393	0.851678
H	-1.236318	-1.552925	0.852387
O	-3.827861	-1.308997	1.013814
O	3.850630	1.688459	1.081697
H	4.519746	1.230065	1.591620
O	1.274543	1.041198	1.154664
H	1.831613	1.576676	1.716850
O	-1.398839	-3.058174	-1.143446
H	-1.648506	-3.701227	-1.796424
H	-0.433087	-2.943764	-1.210290
C	-3.639426	-1.931349	2.259093
H	-2.657227	-2.390517	2.338959
H	-3.767960	-1.219084	3.073964
H	-4.391156	-2.704619	2.339761
C	-2.142897	3.781595	-0.152986
H	-2.910440	4.303046	0.418118
H	-1.170918	4.013682	0.259683
H	-2.181704	4.114525	-1.189157

2D-PC (E= -1181.50737937)

Sum of electronic and zero-point Energies=	-1181.130503
Sum of electronic and thermal Energies=	-1181.107044
Sum of electronic and thermal Enthalpies=	-1181.106100
Sum of electronic and thermal Free Energies=	-1181.186396

O	5.102501	-0.916604	-0.621477
C	5.052211	-0.083666	0.501470
H	5.784089	0.720397	0.413013
H	5.278790	-0.651529	1.407453
C	3.675401	0.516578	0.628003
H	3.598819	1.024090	1.584653
O	3.491309	1.462819	-0.423038
C	2.261731	1.286481	-1.038451
H	2.374595	1.572634	-2.078056
N	-1.657163	0.139204	-0.612979
C	-2.603271	-0.911551	-0.866665
H	-2.466286	-1.250360	-1.891160
C	-4.060761	-0.461433	-0.703152
C	-4.483054	0.489208	-1.818562
H	-4.433670	-0.041771	-2.763006
H	-5.505801	0.814634	-1.660967
H	-3.839432	1.360117	-1.875113
C	-4.213609	0.238882	0.636066
O	-5.212181	0.143132	1.296729
N	-3.150842	1.012489	0.984224
H	-3.209164	1.572083	1.814253
C	-1.945406	0.961413	0.299270
O	-1.134666	1.900050	0.726335
C	2.527084	-0.494905	0.522614
H	2.905231	-1.514269	0.532223
C	1.885275	-0.162052	-0.824869
H	2.354478	-0.754902	-1.602106
H	0.814465	-0.318600	-0.848064
O	1.678303	-0.301936	1.624291
O	-4.870010	-1.607597	-0.704850
H	-5.580669	-1.464134	-0.080052
O	-2.327644	-1.962829	0.024091
H	-3.042072	-2.592016	-0.052613
O	1.283905	2.123410	-0.442683
H	1.640619	3.004682	-0.378592
H	-0.263414	1.837762	0.292886
C	0.770177	-1.351890	1.842935
H	0.067602	-1.470642	1.023106
H	1.298952	-2.293433	1.998700
H	0.217211	-1.108941	2.741544
C	6.374361	-1.439625	-0.872497
H	6.729732	-2.041432	-0.034832
H	6.301673	-2.068317	-1.750806
H	7.097332	-0.646086	-1.063349

Table S1.Comparison of the bond lengths (Å) between crystal structure and theoretical geometry optimized at the BHandHLYP/6-311++G(d,p) level of deoxythymidine glycol.

Bonds	Crystal structure	BHandHLYP/6-311++G(d,p)	
		I[a]	II[b]
N1-C2	1.347	1.364	0.013
C2-O2	1.241	1.200	-0.033
C2-N3	1.390	1.395	0.004
N3-C4	1.415	1.358	-0.040
C4-O4	1.201	1.200	-0.001
C4-C5	1.518	1.518	0.000
C5-O5	1.442	1.401	-0.028
C5-M	1.511	1.523	0.008
C5-C6	1.516	1.527	0.007
C6-O6	1.425	1.403	-0.015
N1-C6	1.432	1.435	0.002
N1-C1’	1.450	1.450	0.000
C1’-O4’	1.427	1.416	-0.008
C1’-C2’	1.507	1.537	0.020
C2’-C3’	1.509	1.524	0.010
C3’-O3’	1.436	1.405	-0.022
C3’-C4’	1.535	1.519	-0.010
C4’-O4’	1.444	1.416	-0.019
C4’-C5’	1.515	1.510	-0.003
C5’-O5’	1.414	1.406	-0.006

[a] Optimized geometry parameters. [b] Relative deviation between the crystal and optimized geometry .

Table S2. Comparison of the bond angles (degree) between crystal structure and theoretical geometry optimized at the BHandHLYP/6-311++G(d,p) level of deoxythymidine glycol.

Bond angles	Crystal structure	BHandHLYP/6-311++G(d,p)	
		I[a]	II[b]
(a) C6-N1-C2	120.3	121.3	0.008
N1-C2-N3	117.5	115.4	-0.018
C2-N3-C4	124.6	127.1	0.020
N3-C4-C5	113.4	115.0	0.014
C4-C5-C6	108.9	108.6	-0.003
C5-C6-N1	110.5	110.6	0.001
(b)C1'-N1-C2	119.3	118.0	-0.011
C1'-N1-C6	120.3	119.4	-0.007
O2-C2-N1	124.0	125.1	0.009
O2- C2-N3	118.5	119.5	0.008
O4-C4-N3	120.4	123.5	0.026
O4-C4-C5	126.1	121.4	-0.037
(c) M-C5-C4	110.7	109.8	-0.008
M-C5-C6	112.8	112.2	-0.005
M-C5-O5	111.0	110.6	-0.004
O5-C5-C4	109.6	108.4	-0.011
O5-C5-C6	103.7	106.9	0.031
O6-C6-N1	106.7	109.3	0.024
O6-C6-C5	111.2	110.3	-0.008
(d) O4' -C1'- C2'	104.8	106.2	0.013
C1'-C2'-C3'	102.0	104.2	0.022
C2'-C3'-C4'	104.5	102.0	-0.024
C3'-C4'-O4'	105.0	104.5	-0.005
C4'-O4'-C1'	110.2	110.2	0.000
N1-C1'-C2'	117.4	115.7	-0.014
N1-C1'-O4'	107.0	108.1	0.010
O3'-C3'-C2'	109.3	114.8	0.050
O3'-C3'-C4'	111.1	108.7	-0.022
C5'-C4'-C3'	114.8	115.9	0.010
C5'-C4'-O4'	110.0	108.8	-0.011
O5'-C5'-C4'	112.3	112.3	0.000

[a] Optimized geometry parameters. [b] Relative deviation between the crystal and optimized geometry .

Table S3. Comparison of the torsion angles (degree) between crystal structure and theoretical geometry optimized at the BHandHLYP/6-311++G(d,p) level of deoxythymidine glycol.

torsion angles	Crystal structure	BHandHLYP/6-311++G(d,p)	
		I[a]	II[b]
O4'-C1'-N1-C2 (χ)	-111.6	-128.2	0.140
O4'-C1'-N1-C6 (χ′)	67.6	63.7	-0.050

[a] Optimized geometry parameters. [b] Relative deviation between the crystal and optimized geometry .