Reliable Vibrational Wavenumbers for C=O and N-H Stretchings of Isolated and Hydrogen-bonded Nucleic Acid Bases
Supplementary Information

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Table. Cartesian coordinates of the optimized structures of the hydrogen-bonded nucleobases dimers, computed at B3LYP-D3/N07D and B2PLYP-D3/maug-cc-pVTZ levels of theory.

U-U1	B3LYP-D3/N07D			B2PLYP-D3/maug-cc-pVTZ		
C	3.0509105	1.0426897	0.0000597	1.5516540	2.8275740	0.0000000
C	-3.0509105	-1.0426897	-0.0000597	-1.5516540	-2.8275740	0.0000000
C	1.7507214	-1.0737016	0.0000961	2.0124660	0.3951030	0.0000000
C	-1.7507214	1.0737016	-0.0000961	-2.0124660	-0.3951030	0.0000000
C	3.0066941	-1.8096633	-0.0000349	3.4298940	0.6948400	0.0000000
C	-3.0066941	1.8096633	0.0000349	-3.4298940	-0.6948400	0.0000000
C	4.1750301	-1.1267444	-0.0001124	3.8318230	1.9803450	0.0000000
C	-4.1750301	1.1267444	0.0001124	-3.8318230	-1.9803450	0.0000000
H	5.1437172	-1.6169368	-0.0002060	4.8725920	2.2668240	0.0000000
H	-5.1437172	1.6169368	0.0002060	-4.8725920	-2.2668240	0.0000000
H	5.0722695	0.7560994	-0.0001991	3.2344350	3.9694790	0.0000000
H	-5.0722695	-0.7560994	0.0001991	-3.2344350	-3.9694790	0.0000000
H	0.9919281	0.8591491	0.0002528	0.1602720	1.3095460	0.0000000
H	-0.9919281	-0.8591491	-0.0002528	-0.1602720	-1.3095460	0.0000000
H	2.9679247	-2.8907977	-0.0000462	4.1280380	-0.1233930	0.0000000
H	-2.9679247	2.8907977	0.0000462	-4.1280380	0.1233930	0.0000000
N	4.2006401	0.2444138	-0.0000452	2.9323900	3.0098020	0.0000000
N	-4.2006401	-0.2444138	0.0000452	-2.9323900	-3.0098020	0.0000000
N	1.8733537	0.3154122	0.0002519	1.1721870	1.5008870	0.0000000
N	-1.8733537	-0.3154122	-0.0002519	-1.1721870	-1.5008870	0.0000000
O	3.1117047	2.2554590	-0.0000093	0.7790090	3.7628190	0.0000000
O	-3.1117047	-2.2554590	0.0000093	-0.7790090	-3.7628190	0.0000000
O	0.6407254	-1.6077516	0.0001145	1.5516540	-0.7460610	0.0000000
O	-0.6407254	1.6077516	-0.0001145	-1.5516540	0.7460610	0.0000000
U-U2						
C	-2.1174587	-0.7729033	0.0000057	-2.0534150	0.9170680	0.0000000
C	-4.4997968	0.0228530	-0.0000059	-3.2098160	3.1365300	0.0000000
C	-3.9800691	1.3840146	-0.0000060	-1.8966720	3.7514720	0.0000000
C	-2.6407189	1.5886992	-0.0000007	-0.7966530	2.9714760	0.0000000
H	-2.1993851	2.5806688	-0.0000006	0.2035050	3.3780180	0.0000000
H	-0.7264999	0.7548545	0.0000095	0.0000000	1.0511470	0.0000000
H	-3.7989964	-1.9282580	0.0000008	-4.0571830	1.2547520	0.0000000
H	-4.6881604	2.2022162	-0.0000105	-1.8334840	4.8254460	0.0000000
N	-1.7372298	0.5565262	0.0000046	-0.8612680	1.6053430	0.0000000
N	-3.4872544	-0.9635062	-0.0000005	-3.1662800	1.7301470	0.0000000
O	-1.3163475	-1.6988760	0.0000115	-2.1233220	-0.3040540	0.0000000
O	-5.6742874	-0.3066560	-0.0000100	-4.2822610	3.7159810	0.0000000
C	4.4281726	0.2937390	-0.0000046	3.3713550	-2.8598700	0.0000000
C	1.9372785	0.5148098	0.0000065	1.7468770	-0.9702330	0.0000000
C	1.8395004	-0.9336489	0.0000033	0.6715240	-1.9352910	0.0000000
C	2.9773011	-1.6671915	-0.0000037	0.9742120	-3.2484370	0.0000000
H	2.9703332	-2.7525281	-0.0000067	0.2154860	-4.0159520	0.0000000
H	5.0654303	-1.6407515	-0.0000131	2.4797500	-4.6828080	0.0000000
H	3.3458427	2.0267854	0.0000049	3.8010990	-0.8700880	0.0000000
H	0.8524091	-1.3853370	0.0000062	-0.3467330	-1.5773930	0.0000000
N	4.2223552	-1.0824349	-0.0000076	2.2690620	-3.6985540	0.0000000
N	3.2424053	1.0176146	0.0000023	3.0266300	-1.5189650	0.0000000
O	5.5304049	0.8023627	-0.0000083	4.5155830	-3.2616230	0.0000000
O	0.9895391	1.3023041	0.0000126	1.6170090	0.2540450	0.0000000
U-U3						
N	-1.9651002	0.2881673	0.0000216	-0.8940650	1.7732580	0.0000000
H	-1.0200597	0.7132330	0.0000508	0.0000000	1.2612810	0.0000000
C	-2.0408520	-1.1011706	0.0000290	-2.0564100	1.0175670	0.0000000
O	-1.0153547	-1.7907591	0.0000639	-2.0091860	-0.2157740	0.0000000
C	-3.3846853	-1.6546925	-0.0000075	-3.2892560	1.7742640	0.0000000
H	-3.4981308	-2.7304759	-0.0000025	-4.2226320	1.2397380	0.0000000
C	-4.4471787	-0.8150822	-0.0000479	-3.2364040	3.1207420	0.0000000
H	-5.4743997	-1.1662960	-0.0000774	-4.1208020	3.7396220	0.0000000
N	-4.2813704	0.5445142	-0.0000544	-2.0451810	3.7876600	0.0000000
H	-5.0732513	1.1731119	-0.0000852	-2.0079930	4.7934320	0.0000000
C	-3.0314486	1.1746870	-0.0000193	-0.8055760	3.1530310	0.0000000
O	-2.9194520	2.3822002	-0.0000272	0.2360760	3.7717990	0.0000000
N	2.9701859	1.0320703	0.0000231	2.6023680	-1.8072190	0.0000000
H	3.0606543	2.0422725	0.0000411	3.4685280	-1.2871700	0.0000000
C	4.1754247	0.2896696	-0.0000318	2.7132380	-3.2115730	0.0000000
O	5.2482286	0.8680843	-0.0000543	3.8117830	-3.7376340	0.0000000
C	3.9646882	-1.1522102	-0.0000573	1.4304950	-3.8878990	0.0000000

H	4.8349523	-1.7952981	-0.0000996	1.4183170	-4.9637890	0.0000000
C	2.7030187	-1.6458533	-0.0000283	0.2937870	-3.1628620	0.0000000
H	2.4900195	-2.7103618	-0.0000453	-0.6851930	-3.6177360	0.0000000
N	1.5965352	-0.8345920	0.0000251	0.2946200	-1.7949010	0.0000000
H	0.6384099	-1.2256468	0.0000458	-0.5803850	-1.2558770	0.0000000
C	1.6834331	0.5397301	0.0000519	1.4514660	-1.0582670	0.0000000
O	0.6951096	1.2724506	0.0000983	1.4635690	0.1702200	0.0000000
U-U4						
O	-1.0040087	-1.4614515	0.0000000	-1.4681590	0.9909130	0.0000000
C	-1.9148905	-0.6284486	0.0000000	-0.6404970	1.9048300	0.0000000
N	-1.6891390	0.7276144	0.0000000	0.7109040	1.6888720	0.0000000
C	-2.7101771	1.6469100	0.0000000	1.6182750	2.7150210	0.0000000
C	-4.0142772	1.2822522	0.0000000	1.2464310	4.0105560	0.0000000
C	-4.3686137	-0.1309420	0.0000000	-0.1624910	4.3530550	0.0000000
N	-3.2410014	-0.9905577	0.0000000	-1.0093930	3.2240290	0.0000000
O	-5.4913701	-0.6020571	0.0000000	-0.6404970	5.4720500	0.0000000
H	-4.8155136	2.0095708	0.0000000	1.9671220	4.8094420	0.0000000
H	-0.6996410	1.0306224	0.0000000	1.0214050	0.7078990	0.0000000
H	-3.4335450	-1.9863647	0.0000000	-2.0025780	3.4084710	0.0000000
H	-2.3903469	2.6841721	0.0000000	2.6526390	2.4065850	0.0000000
O	1.0040087	1.4614515	0.0000000	1.4681590	-0.9909130	0.0000000
C	1.9148905	0.6284486	0.0000000	0.6404970	-1.9048300	0.0000000
N	1.6891390	-0.7276144	0.0000000	-0.7109040	-1.6888720	0.0000000
C	2.7101771	-1.6469100	0.0000000	-1.6182750	-2.7150210	0.0000000
C	4.0142772	-1.2822522	0.0000000	-1.2464310	-4.0105560	0.0000000
C	4.3686137	0.1309420	0.0000000	0.1624910	-4.3530550	0.0000000
N	3.2410014	0.9905577	0.0000000	1.0093930	-3.2240290	0.0000000
O	5.4913701	0.6020571	0.0000000	0.6404970	-5.4720500	0.0000000
H	4.8155136	-2.0095708	0.0000000	-1.9671220	-4.8094420	0.0000000
H	0.6996410	-1.0306224	0.0000000	-1.0214050	-0.7078990	0.0000000
H	3.4335450	1.9863647	0.0000000	2.0025780	-3.4084710	0.0000000
H	2.3903469	-2.6841721	0.0000000	-2.6526390	-2.4065850	0.0000000
U-U5						
O	-3.0993365	-2.2596404	-0.0000516	0.2904440	3.8231680	0.0000000
C	-3.0465902	-1.0461285	-0.0000367	1.1796760	2.9974340	0.0000000
N	-4.1995863	-0.2540222	-0.0000831	2.5242490	3.3575780	0.0000000
C	-4.1803305	1.1178112	-0.0000642	3.5500690	2.4531980	0.0000000
C	-3.0157812	1.8069044	0.0000064	3.3192220	1.1263560	0.0000000
C	-1.7552774	1.0782934	0.0000555	1.9530220	0.6436130	0.0000000
N	-1.8731485	-0.3125680	0.0000360	0.9765600	1.6328300	0.0000000
O	-0.6480182	1.6153683	0.0001300	1.6428460	-0.5463050	0.0000000
H	-2.9830328	2.8882575	0.0000262	4.1182470	0.4062870	0.0000000
H	-5.0689989	-0.7694583	-0.0001363	2.6994540	4.3482880	0.0000000
H	-0.9921467	-0.8516360	0.0000793	0.0000000	1.3133640	0.0000000
H	-5.1515078	1.6029775	-0.0001064	4.5446360	2.8727770	0.0000000
O	0.6711345	-1.5824724	0.0001263	-1.6304940	0.5070910	0.0000000
C	1.7536257	-1.0002935	0.0000608	-1.8932350	-0.6921700	0.0000000
N	2.9436367	-1.7143397	0.0000078	-3.2029310	-1.1308040	0.0000000
C	4.1838676	-1.1142801	-0.0000661	-3.5492020	-2.4593650	0.0000000
C	4.3126247	0.2298391	-0.0000908	-2.6157580	-3.4264890	0.0000000
C	3.1196196	1.0782815	-0.0000352	-1.2028040	-3.0727590	0.0000000
N	1.9018281	0.3613248	0.0000376	-0.9579290	-1.6869620	0.0000000
O	3.1227382	2.2953463	-0.0000572	-0.2805460	-3.8659260	0.0000000
H	5.2802104	0.7144930	-0.0001502	-2.8789280	-4.4697710	0.0000000
H	2.8420434	-2.7198204	0.0000245	-3.8996970	-0.4052110	0.0000000
H	1.0221698	0.9051240	0.0000796	0.0214380	-1.3726790	0.0000000
H	5.0318148	-1.7918051	-0.0001028	-4.6087130	-2.6646810	0.0000000
U-U6						
O	2.7454317	2.4033244	0.0000117	-0.8901960	3.5413480	0.0000000
C	2.9973804	1.2146242	0.0000120	0.2791220	3.2154280	0.0000000
N	4.3139816	0.7403131	0.0000548	1.3054640	4.1569150	0.0000000
C	4.6426893	-0.5920343	0.0000583	2.6333110	3.8288630	0.0000000
C	3.6904360	-1.5525514	0.0000200	3.0409820	2.5459100	0.0000000
C	2.2815710	-1.1717458	-0.0000257	2.0546760	1.4798070	0.0000000
N	2.0465797	0.2098221	-0.0000267	0.7274080	1.9113590	0.0000000
O	1.3475931	-1.9664759	-0.0000615	2.3249840	0.2845900	0.0000000
H	3.9348615	-2.6065402	0.0000223	4.0830560	2.2789580	0.0000000
H	5.0237558	1.4596092	0.0000839	1.0020610	5.1159580	0.0000000
H	1.0625297	0.5211388	-0.0000602	0.0000000	1.1865720	0.0000000
H	5.7052196	-0.8153015	0.0000935	3.3213710	4.6607420	0.0000000

O	-0.6919355	1.0830995	-0.0000990	-1.3010420	-0.1221160	0.0000000
C	-1.7046838	0.3888916	-0.0000507	-1.1534330	-1.3400550	0.0000000
N	-2.9621298	1.0110543	-0.0000221	-2.2804270	-2.1653080	0.0000000
C	-4.2079094	0.4012655	0.0000285	-2.3161500	-3.5470770	0.0000000
N	-4.1320682	-0.9882413	0.0000516	-1.0545560	-4.1191110	0.0000000
C	-2.9458597	-1.6879740	0.0000275	0.1087050	-3.3908320	0.0000000
C	-1.7454009	-1.0645899	-0.0000227	0.1107640	-2.0442800	0.0000000
O	-5.2608302	1.0080290	0.0000506	-3.3408210	-4.1980740	0.0000000
H	-0.8016035	-1.5994590	-0.0000410	1.0184760	-1.4619200	0.0000000
H	-5.0236819	-1.4644666	0.0000888	-1.0410480	-5.1252040	0.0000000
H	-2.9684263	2.0255197	-0.0000410	-3.1791440	-1.7035680	0.0000000
H	-3.0422065	-2.7691014	0.0000509	1.0187360	-3.9710950	0.0000000
A-A						
N	-1.2746370	1.3765840	0.0000390	1.0820670	1.5393510	0.0000000
C	-2.1234380	0.3388270	0.0000070	2.0603540	0.6269180	0.0000000
N	-1.6389260	-0.9271410	-0.0000370	1.7542920	-0.6874730	0.0000000
C	-2.5008720	-1.9604160	-0.0000690	2.7503400	-1.5892810	0.0000000
N	-3.8334370	-1.9341490	-0.0000620	4.0632960	-1.3798300	0.0000000
C	-4.2943090	-0.6741310	-0.0000160	4.3410700	-0.0702130	0.0000000
C	-3.5316170	0.4980320	0.0000200	3.4253930	0.9771200	0.0000000
N	-4.3369240	1.6229700	0.0000620	4.0632960	2.2028490	0.0000000
C	-5.5576100	1.1439270	0.0000460	5.3376760	1.8974940	0.0000000
N	-5.5993440	-0.2371980	0.0000050	5.5700400	0.5420400	0.0000000
H	-2.0419740	-2.9477550	-0.0001040	2.4348680	-2.6248650	0.0000000
H	-6.4630480	1.7379120	0.0000680	6.1461010	2.6085900	0.0000000
H	-6.4199470	-0.8263320	-0.0000110	6.4607470	0.0755700	0.0000000
H	-0.2529410	1.2359900	0.0000020	0.0961490	1.2626230	0.0000000
H	-1.6597640	2.3087260	0.0000620	1.3398860	2.5098090	0.0000000
N	1.2746440	-1.3765970	0.0000390	-1.0820670	-1.5393510	0.0000000
C	2.1234410	-0.3388360	0.0000070	-2.0603540	-0.6269180	0.0000000
N	1.6389210	0.9271290	-0.0000370	-1.7542920	0.6874730	0.0000000
C	2.5008600	1.9604100	-0.0000680	-2.7503400	1.5892810	0.0000000
N	3.8334250	1.9341520	-0.0000620	-4.0632960	1.3798300	0.0000000
C	4.2943040	0.6741360	-0.0000170	-4.3410700	0.0702130	0.0000000
C	3.5316210	-0.4980320	0.0000200	-3.4253930	-0.9771200	0.0000000
N	4.3369350	-1.6229650	0.0000590	-4.0632960	-2.2028490	0.0000000
C	5.5576180	-1.1439140	0.0000510	-5.3376760	-1.8974940	0.0000000
N	5.5993430	0.2372120	0.0000030	-5.5700400	-0.5420400	0.0000000
H	2.0419550	2.9477460	-0.0001040	-2.4348680	2.6248650	0.0000000
H	6.4630610	-1.7378920	0.0000750	-6.1461010	-2.6085900	0.0000000
H	6.4199420	0.8263510	-0.0000140	-6.4607470	-0.0755700	0.0000000
H	0.2529490	-1.2360050	0.0000030	-0.0961490	-1.2626230	0.0000000
H	1.6597730	-2.3087380	0.0000610	-1.3398860	-2.5098090	0.0000000
A-U						
N	4.2493620	-1.0889050	0.0000940	4.2549800	1.0758840	-0.0005810
C	4.8699700	0.1356660	0.0001330	4.8624090	-0.1501790	-0.0007990
C	4.1590920	1.2875310	0.0001020	4.1472480	-1.2919490	-0.0004360
C	2.7025410	1.2270050	0.0000220	2.6983670	-1.2217490	0.0002000
N	2.1639300	-0.0572760	-0.0000100	2.1720130	0.0622360	0.0004090
C	2.8600320	-1.2462360	0.0000280	2.8738000	1.2435320	-0.0000090
O	1.9657460	2.2143570	-0.0000160	1.9551010	-2.2025200	0.0005440
O	2.3357890	-2.3463820	-0.0000150	2.3560180	2.3450560	0.0000900
N	-0.6353290	-0.3015800	-0.0001030	-0.6423230	0.3059450	0.0007670
C	-1.4662300	0.7668180	-0.0000510	-1.4698620	-0.7578960	0.0003880
C	-2.8570720	0.5040390	-0.0000160	-2.8534700	-0.4991590	-0.0000600
C	-3.2359750	-0.8435430	-0.0000390	-3.2367720	0.8394870	-0.0000600
N	-2.4250710	-1.9123120	-0.0000890	-2.4328560	1.9098770	0.0003110
C	-1.1428230	-1.5502690	-0.0001170	-1.1531520	1.5505140	0.0006980
N	-3.9606370	1.3383380	0.0000470	-3.9518020	-1.3375810	-0.0005490
C	-4.9830580	0.5173560	0.0000500	-4.9750500	-0.5193580	-0.0007610
N	-4.6117420	-0.8135120	-0.0000030	-4.6092710	0.8065840	-0.0004930
N	-0.9492660	2.0055790	-0.0000360	-0.9560470	-1.9944920	0.0004830
H	-0.3985580	-2.3445880	-0.0001550	-0.4167000	2.3438270	0.0009850
H	-6.0242500	0.8149240	0.0000880	-6.0091820	-0.8189210	-0.0011240
H	-5.2194100	-1.6205660	-0.0000110	-5.2168620	1.6077420	-0.0006950
H	0.0640420	2.1487900	-0.0000290	0.0512810	-2.1367840	0.0004980
H	-1.5756340	2.7954260	0.0000280	-1.5830510	-2.7780270	-0.0000630
H	4.7792490	-1.9495510	0.0001150	4.7914390	1.9270090	-0.0009020
H	1.1137010	-0.1433150	-0.0000560	1.1305550	0.1532520	0.0007030
H	5.9554030	0.1135870	0.0001880	5.9418240	-0.1376770	-0.0012770

H	4.6355780	2.2589760	0.0001310	4.6177740	-2.2593250	-0.0006070
A-ThioU						
N	-2.3001860	0.4504350	0.0000000	-2.2982330	0.4840420	0.0000000
C	-1.2678370	1.3084850	0.0000000	-1.2556550	1.3251060	0.0000000
N	0.0000000	0.8342700	0.0000000	0.0000000	0.8352410	0.0000000
C	1.0331970	1.7047360	0.0000000	1.0413790	1.6919300	0.0000000
N	0.9856440	3.0369360	0.0000000	1.0108930	3.0214230	0.0000000
C	-0.2775800	3.4856490	0.0000000	-0.2453290	3.4809130	0.0000000
C	-1.4428810	2.7125600	0.0000000	-1.4122350	2.7233300	0.0000000
N	-2.5760610	3.5067510	0.0000000	-2.5360130	3.5276950	0.0000000
C	-2.1080920	4.7316400	0.0000000	-2.0529560	4.7456670	0.0000000
N	-0.7272760	4.7863940	0.0000000	-0.6779690	4.7840740	0.0000000
H	2.0165300	1.2424710	0.0000000	2.0141920	1.2212030	0.0000000
H	-2.7106440	5.6313980	0.0000000	-2.6422540	5.6467140	0.0000000
H	-0.1455060	5.6122910	0.0000000	-0.0899470	5.5996870	0.0000000
H	-2.1354450	-0.5568400	0.0000000	-2.1462720	-0.5190660	0.0000000
H	-3.2412540	0.8121040	0.0000000	-3.2285960	0.8604180	0.0000000
S	-1.5997210	-2.8858480	0.0000000	-1.6096920	-2.8603910	0.0000000
C	0.0776260	-3.0070880	0.0000000	0.0478700	-3.0045740	0.0000000
N	0.8986550	-1.8983290	0.0000000	0.8817200	-1.9102650	0.0000000
C	2.2846910	-1.9065720	0.0000000	2.2629270	-1.9342440	0.0000000
N	2.8505450	-3.1806980	0.0000000	2.8093050	-3.2097630	0.0000000
C	2.1076130	-4.3328680	0.0000000	2.0525900	-4.3480310	0.0000000
C	0.7526760	-4.2836450	0.0000000	0.7048550	-4.2843910	0.0000000
O	2.9715120	-0.9014680	0.0000000	2.9590890	-0.9367030	0.0000000
H	0.1575120	-5.1867850	0.0000000	0.1031700	-5.1759190	0.0000000
H	3.8614270	-3.1994910	0.0000000	3.8152450	-3.2442730	0.0000000
H	0.4783970	-0.9345100	0.0000000	0.4714040	-0.9502050	0.0000000
H	2.6666890	-5.2630290	0.0000000	2.5968340	-5.2800450	0.0000000
A-T						
N	-3.8321870	1.5962860	0.0000670	-3.8428160	1.5817090	0.0010100
C	-4.5577770	0.4254560	0.0001130	-4.5540380	0.4072830	0.0013600
C	-3.9659610	-0.7938810	0.0001160	-3.9538490	-0.8006010	0.0006670
C	-2.5002380	-0.8363270	0.0000700	-2.4960820	-0.8316170	-0.0004550
N	-1.8518440	0.3913580	0.0000240	-1.8610170	0.3975840	-0.0008080
C	-2.4404530	1.6382160	0.0000190	-2.4579550	1.6363460	-0.0001060
C	-4.7169750	-2.0930560	0.0001660	-4.6930190	-2.0999020	0.0010450
O	-1.8524870	-1.8865710	0.0000700	-1.8410180	-1.8758660	-0.0010860
O	-1.8177740	2.6872260	-0.0000220	-1.8433290	2.6882730	-0.0002320
N	0.9608660	0.3878770	-0.0000560	0.9668060	0.3924350	-0.0017000
C	1.6942560	-0.7493550	-0.0000480	1.6974910	-0.7397340	-0.0011050
C	3.1027920	-0.6104420	-0.0000630	3.0985990	-0.6039000	0.0000070
C	3.5988230	0.6986770	-0.0000840	3.5977180	0.6960390	0.0002490
N	2.8853440	1.8346760	-0.0000920	2.8910580	1.8328790	-0.0003430
C	1.5759520	1.5870650	-0.0000770	1.5846940	1.5874360	-0.0012660
N	4.1287650	-1.5386270	-0.0000590	4.1193180	-1.5353230	0.0008910
C	5.2194530	-0.8107360	-0.0000760	5.2102070	-0.8098840	0.0018400
N	4.9666860	0.5476080	-0.0000910	4.9622230	0.5430260	0.0013490
N	1.0693130	-1.9375760	-0.0000290	1.0766840	-1.9264840	-0.0017710
H	0.9041380	2.4435510	-0.0000810	0.9203280	2.4420580	-0.0017020
H	6.2304130	-1.1987720	-0.0000780	6.2140250	-1.1991480	0.0027260
H	5.6429510	1.2981030	-0.0001050	5.6376100	1.2879000	0.0019880
H	0.0471500	-1.9894300	-0.0000010	0.0606190	-1.9790620	-0.0015690
H	1.6230000	-2.7799220	-0.0000110	1.6323270	-2.7621160	-0.0005710
H	-4.2907710	2.4967210	0.0000640	-4.3095460	2.4728320	0.0015420
H	-0.7991560	0.3835020	-0.0000100	-0.8164700	0.3965640	-0.0013610
H	-5.6372510	0.5466050	0.0001460	-5.6288370	0.5165580	0.0022710
H	-4.4538720	-2.6925470	-0.8785490	-4.4279140	-2.6931680	-0.8731270
H	-4.4538130	-2.6925130	0.8788870	-4.4265940	-2.6934240	0.8746440
H	-5.7985430	-1.9254540	0.0001990	-5.7691700	-1.9378230	0.0018870
G-C						
C	-2.9287370	1.0631030	-0.0000050	-2.9225060	1.0603640	-0.0420490
N	-4.3301240	0.9096130	-0.0000150	-4.3166130	0.9094700	-0.0496430
C	-4.9331320	-0.3113230	-0.0000120	-4.9197630	-0.3058790	-0.0226000
C	-4.1827610	-1.4429730	0.0000020	-4.1761180	-1.4337860	0.0135720
C	-2.7455640	-1.2803320	0.0000150	-2.7471450	-1.2741470	0.0213580
N	-2.1757630	-0.0671170	0.0000120	-2.1741740	-0.0691190	-0.0031180
O	-2.4643810	2.2059720	-0.0000120	-2.4537740	2.1995330	-0.0708530
N	-1.9399490	-2.3455700	0.0000370	-1.9481800	-2.3396440	0.0544210
H	-4.8666350	1.7670830	-0.0000230	-4.8510160	1.7624700	-0.0780730

Coordinates

H	-6.0185740	-0.3197800	-0.0000220	-5.9990400	-0.3117550	-0.0320180
H	-4.6432900	-2.4237530	0.0000050	-4.6374470	-2.4070010	0.0345420
H	-2.3298810	-3.2747410	0.0000170	-2.3443750	-3.2610260	0.0663780
H	-0.9061630	-2.2303550	0.0000220	-0.9216270	-2.2274610	0.0428290
O	0.8090640	-2.0293310	-0.0000230	0.8043020	-2.0219160	0.0066960
C	1.4260500	-0.9551700	-0.0000130	1.4231190	-0.9507350	0.0113070
N	0.7147710	0.2592610	-0.0000040	0.7204990	0.2621720	0.0399910
C	1.2709440	1.5176060	0.0000060	1.2768980	1.5138340	0.0499860
N	2.5795960	1.7337330	0.0000100	2.5792160	1.7292880	0.0254850
C	3.2934960	0.5911140	0.0000030	3.2865170	0.5839640	-0.0029830
C	2.8396840	-0.7350360	-0.0000090	2.8310440	-0.7329950	-0.0101890
N	3.9016680	-1.6233570	-0.0000130	3.8883970	-1.6231260	-0.0418780
C	4.9653390	-0.8647780	-0.0000040	4.9516340	-0.8656690	-0.0535210
N	4.6608950	0.4898780	0.0000060	4.6501670	0.4825560	-0.0313030
N	0.4147900	2.5610890	0.0000130	0.4203570	2.5531970	0.1063450
H	-0.3178850	0.1679610	-0.0000010	-0.3062670	0.1761070	0.0408650
H	5.9901240	-1.2142550	-0.0000040	5.9693410	-1.2155350	-0.0777040
H	5.3054730	1.2673520	0.0000150	5.2924600	1.2557800	-0.0331560
H	0.8187010	3.4835820	0.0000270	0.8211640	3.4693150	0.0322580
H	-0.6024370	2.4477990	0.0000080	-0.5871820	2.4348970	0.0259470

Table. Structural parameters of the hydrogen-bonded nucleobases dimers optimized at B3LYP-D3/N07D and B2PLYP-D3/maug-cc-pVTZ levels of theory.

	B3LYP-D3/N07D	B2PLYP-D3/maug-cc-pVTZ
U-U1		
r N3-H3(M1)	1.0357	1.0299
r N3(M1)-O4(M2)	2.8268	2.8265
r H3(M1)-O4(M2)	1.7961	1.8023
r N3-H3(M2)	1.0357	1.0299
r N3(M2)-O4(M1)	2.8268	2.8265
r H3(M2)-O4(M1)	1.7961	1.8023
U-U2		
r N1-H1(M1)	1.0300	1.0242
r N1(M1)-O4(M2)	2.8269	2.8227
r H1(M1)-O4(M2)	1.8013	1.8028
U-U3		
r N3-H3(M1)	1.0362	1.0303
r N3(M1)-O2(M2)	2.8365	2.8510
r H3(M1)-O2(M2)	1.8040	1.8255
r N1-H1(M2)	1.0349	1.0277
r N1(M2)-O4(M1)	2.7814	2.7931
r H1(M2)-O4(M1)	1.7477	1.7673
U-U4		
r N1-H1(M1)	1.0349	1.0289
r N1(M1)-O2(M2)	2.7913	2.7847
r H1(M1)-O2(M2)	1.7573	1.7566
r N1-H1(M2)	1.0349	1.0289
r N1(M2)-O2(M1)	2.7913	2.7847
r H1(M2)-O2(M1)	1.7573	1.7566
U-U5		
r N3-H3(M1)	1.0342	1.0286
r N3(M1)-O4(M2)	2.8415	2.8399
r H3(M1)-O4(M2)	1.8149	1.8199
r N3-H3(M2)	1.0328	1.0275
r N3(M2)-O2(M1)	2.8436	2.8397
r H3(M2)-O2(M1)	1.8168	1.8190
U-U6		
r N3-H3(M1)	1.0321	1.0269
r N3(M1)-O4(M2)	2.8744	2.8722
r H3(M1)-O4(M2)	1.8423	1.8454
A-A		
r N6-Ha(M1)	1.0313	1.0240
r N6(M1)-N1(M2)	2.9480	2.9615
r Ha(M1)-N1(M2)	1.9169	1.9378
r N6-Ha(M2)	1.0313	1.0240
r N6(M2)-N1(M1)	2.9480	2.9615
r Ha(M2)-N1(M1)	1.9169	1.9378
A-U		
r N6-Ha(A)	1.0234	1.0173
r N6(A)-O4(U)	2.9225	2.9186
r Ha(A)-O4(U)	1.9028	1.9050
r N3-H3(U)	1.0538	1.0454
r N3(U)-N1(A)	2.8099	2.8249
r H3(U)-N1(A)	1.7562	1.7794
A-ThioU		
r N3-H3(ThioU)	1.0515	1.0441

r N3(ThioU)-N1(A)	2.8766	2.8836
r H3(ThioU)-N1(A)	1.8323	1.8466
A-T		
r N6-Ha(A)	1.0235	1.0174
r N6(A)-O4(T)	2.9223	2.9181
r Ha(A)-O4(T)	1.9024	1.9044
r N3-H3(T)	1.0527	1.0446
r N3(T)-N1(A)	2.8127	2.8278
r H3(T)-N1(A)	1.7600	1.7833
G-C		
r N2-Ha(G)	1.0235	1.0176
r N2(G)-O2(C)	2.9010	2.9012
r Ha(G)-O2(C)	1.8776	1.8839
r N1-H1(G)	1.0367	1.0304
r N1(G)-N3(C)	2.9089	2.9139
r H1(G)-N3(C)	1.8727	1.8845
r N4-Hb(C)	1.0402	1.0327
r N4(C)-O6(G)	2.7671	2.7712
r Hb(C)-O6(G)	1.7270	1.7385
4APM-M4PMN		
r N4-Ha(4APM)	1.0296	1.0232
r N4(4APM)-O4(M4PMN)	2.8361	2.8342
r Ha(4APM)-O4(M4PMN)	1.8065	1.8111
r N3-H3(M4PMN)	1.0462	1.0387
r N3(M4PMN)-N3(4APM)	2.8782	2.8885
r H3(M4PMN)-N3(4APM)	1.8321	1.8500

Table. Harmonic vibrational frequencies for nucleobases complexes, computed at B2PLYP-D3/maug-cc-pVTZ and B3LYP-D3/N07D levels of theory.

Assignment a	B2PLYP-D3/maug-cc-pVTZ	B3LYP-D3/N07D	
Mode	harm	harm	Δharm
U-U1			
νN1H (M1, M2)	3646	3645	-0.6
νN1H (M1, M2)	3646	3645	-0.6
νC5H (M1,M2)	3268	3262	-6.4
νC5H (M1,M2)	3267	3262	-5.7
νN3H (M1,M2)	3270	3248	-22.6
νC6H (M1,M2)	3223	3216	-7.1
νC6H (M1,M2)	3223	3216	-7.1
νN3H (M1,M2)	3227	3202	-24.5
νC2=O (M1,M2)	1797	1814	17.1
νC2=O (M1,M2)	1795	1812	17.8
νC4=O, ν ring, δN3H (M1,M2)	1731	1743	12.2
νC4=O, ν ring, δN3H (M1,M2)	1722	1734	11.3
νC5=C6 (M1,M2)	1669	1671	1.6
νC5=C6 (M1,M2)	1669	1670	1.6
ν ring, δN1H, δN3H (M1,M2)	1517	1519	2.5
ν ring, δN1H, δN3H (M1,M2)	1516	1518	2.0
δN3H (M1,M2)	1484	1490	6.3
δN3H (M1,M2)	1477	1486	8.3
ν ring, δN1H, δCH (M1,M2)	1428	1421	-6.9
ν ring, δN1H, δCH (M1,M2)	1425	1418	-7.0
U-U2			
νN_1H (M2)	3641	3641	-0.2
νN_3H (M1)	3604	3610	6.2
νN_3H (M2)	3598	3604	6.1
νN_1H (M1)	3311	3292	-19.4
νC_5H (M1)	3265	3259	-6.4
νC_6H (M2)	3232	3226	-6.8
νC_6H (M1)	3223	3217	-6.1
νC_5H (M2)	3214	3207	-7.5
νC_2=O (M2)	1799	1817	17.5
νC_2=O (M1)	1772	1787	14.9
νC_4=O (M1)	1751	1767	15.8
νC_4=O (M2)	1717	1727	10.6
νC_5=C_6 (M1)	1674	1674	0.5
νC_5=C_6 (M2)	1666	1668	2.6
δN_1H (M1)	1564	1566	2.7
δN_1H (M2)	1511	1511	-0.1
ν ring, δN_1H, δCH (M1)	1449	1440	-8.5
ν ring, δN_1H, δCH (M2)	1430	1424	-6.6
δN_3H + δCH (M2)	1425	1422	-2.9
δN_3H + δCH (M1)	1416	1415	-1.3
ν ring, δN3H, δCH (M1,M2)	1393	1392	-1.4
ν ring, δN3H, δCH (M1,M2)	1392	1391	-1.3
δCH, ν ring (M1,M2)	1263	1258	-5.2
δCH, ν ring (M1,M2)	1256	1252	-3.9
U-U3			
νN1H (M1)	3642	3642	-0.6
νN3H (M2)	3599	3606	6.8
νC5H (M1)	3269	3262	-6.4
νC5H (M2)	3265	3259	-6.6
νN3H (M1), νN1H (M2)	3272	3237	-35.1
νC6H (M2)	3226	3218	-7.8
νC6H (M1)	3225	3218	-7.2
νN3H (M1), νN1H (M2)	3227	3186	-41.4
νC2=O (M1)	1801	1820	18.6
νC2=O, νC4=O, ν ring, δN1H (M2)	1765	1782	17.0
νC2=O, νC4=O, δNH (M2)	1750	1764	13.6

νC4=O, ν ring, δN3H (M1)	1718	1728	10.2
νC5=C6 (M2)	1673	1674	0.8
νC5=C6 (M1)	1667	1668	0.7
δN1H (M2)	1558	1568	10.7
ν ring, δN1H, δN3H (M1)	1520	1524	4.3
δN3H (M1)	1480	1493	13.4
ν ring, δN1H, δCH (M2)	1454	1447	-7.1
ν ring, δN1H, δCH (M1)	1428	1422	-5.9
δN3H + δCH (M2)	1421	1417	-4.2
U-U4			
νN3H (M1,M2)	3600	3606	5.9
νN3H (M1,M2)	3600	3606	5.9
νC5H (M1,M2)	3265	3259	-5.9
νC5H (M1,M2)	3265	3259	-5.9
νN1H (M1,M2)	3253	3235	-18.6
νC6H (M1,M2)	3227	3221	-5.6
νC6H (M1,M2)	3227	3221	-6.0
νN1H (M1,M2)	3201	3181	-20.3
νC4=O, ν ring, δN1H (M1,M2)	1771	1788	17.1
νC4=O, ν ring, δN3H (M1,M2)	1763	1783	19.2
νC2=O, ν ring, δNH (M1,M2)	1747	1759	12.2
νC2=O, δN1H (M1,M2)	1746	1755	9.3
νC5=C6 (M1,M2)	1676	1677	1.3
νC5=C6 (M1,M2)	1674	1676	1.8
δN_1H (M1,M2)	1566	1572	6.2
δN_1H (M1,M2)	1565	1567	2.3
ν ring, δN_1H, δCH (M1,M2)	1459	1451	-7.8
ν ring, δN_1H, δCH (M1,M2)	1457	1448	-8.8
δN_3H + δCH (M1,M2)	1424	1418	-5.9
δN_3H + δCH (M1,M2)	1423	1417	-5.8
ν ring, δN3H, δCH (M1,M2)	1396	1400	3.9
ν ring, δN3H, δCH (M1,M2)	1395	1399	3.2
U-U5			
νN_1H (M1)	3648	3647	-1.0
νN_1H (M2)	3646	3645	-0.5
νN3H (M1,M2)	3304	3288	-16.2
νC_5H (M2)	3268	3262	-6.5
νC_5H (M1)	3265	3258	-6.4
νN3H (M1,M2)	3262	3242	-19.8
νC_6H (M1)	3225	3218	-6.9
νC_6H (M2)	3224	3217	-7.0
νC_2=O (M2)	1796	1813	17.3
νC_4=O (M1)	1762	1782	20.3
νC_2=O (M1)	1756	1768	12.2
νC_4=O (M2)	1727	1740	12.5
$\nu C_5=C_6$ (M1)	1678	1680	2.0
$\nu C_5=C_6$ (M2)	1669	1671	1.7
ν ring, δN1H (M2)	1515	1517	1.8
ν ring, δN1H (M1)	1501	1501	-0.2
δN3H + δCH (M1,M2)	1479	1486	6.4
δN3H + δCH (M1,M2)	1474	1483	8.5
ν ring, δN1H (M1)	1430	1423	-6.6
ν ring, δN_1H, δCH (M2)	1426	1419	-6.9
ν ring, δN_1H, δCH (M1)	1412	1402	-9.1
ν ring, δCH (M2)	1398	1390	-8.7
U-U6			
νN_1H (M1)	3648	3647	-0.7
νN_1H (M2)	3645	3645	-0.5
νN_3H (M2)	3598	3604	6.1
νN_3H (M1)	3303	3289	-14.6
νC_5H (M1)	3266	3259	-6.5
νCHsym (M2)	3235	3226	-8.9

νCHasym (M2)	3223	3215	-7.7
νC_6H (M1)	3221	3214	-7.2
νC2=O (M1,M2)	1795	1812	16.9
νC2=O (M1,M2)	1793	1810	17.3
νC4=O, ν ring, δN3H (M1,M2)	1740	1755	14.7
νC4=O, ν ring, δN3H (M1,M2)	1726	1738	12.7
$\nu C_5{=}C_6$ (M1)	1672	1673	1.4
$\nu C_5{=}C_6$ (M2)	1669	1671	2.5
ν ring, δN1H (M1)	1511	1513	1.8
ν ring, δN1H (M2)	1507	1507	-0.1
δN3H + δCH (M1)	1480	1487	6.1
δN3H + δCH (M2)	1428	1422	-5.4
A-A			
$\nu_{asym}NH_2$ (M1,M2)	3680	3679	-1.4
$\nu_{asym}NH_2$ (M1,M2)	3680	3679	-1.3
νN9H (M1,M2)	3658	3657	-0.9
νN9H (M1,M2)	3658	3657	-0.9
νsymNH2 (M1,M2)	3295	3254	-40.9
νsymNH2 (M1,M2)	3255	3210	-45.6
νC8H (M1,M2)	3263	3256	-7.8
νC8H (M1,M2)	3263	3256	-7.8
νC2H (M1,M2)	3183	3173	-9.8
νC2H (M1,M2)	3183	3173	-9.9
δscissNH2, νC5C6, νC6N6 (M1,M2)	1707	1709	2.3
δscissNH2, νC5C6, νC6N6 (M1,M2)	1706	1709	3.2
νC5C6, νC6N6, δscissNH2 (M1,M2)	1655	1654	-0.6
νC5C6, νC6N6, δscissNH2 (M1,M2)	1639	1638	-1.1
νN3C4, νC5C6 (M1,M2)	1624	1630	5.8
δscissNH2, νC4C5, νC5C6 (M1,M2)	1626	1629	3.5
δscissNH2, νC6N6 (M1,M2)	1532	1534	1.7
νN7C8, δC8H (M1,M2)	1525	1530	5.2
νN7C8, δC8H (M1,M2)	1508	1516	8.6
νN1C6, δC2H, νC2N3, νC6N6 (M1,M2)	1501	1507	6.0
νC4C5, νC4N9, δC2H (M1,M2)	1450	1450	0.5
νC4C5, νC4N9, δC2H (M1,M2)	1449	1449	0.6
δN9H, δC2H, νC4N9, νC8N9 (M1,M2)	1423	1422	-0.8
δN9H, δC2H, νC4N9, νC8N9 (M1,M2)	1422	1421	-1.0
δC2H, νC8N9, δC8H, νC6N6 (M1,M2)	1382	1377	-5.2
δC2H, νC8N9, δC8H, νC6N6 (M1,M2)	1382	1376	-5.7
νN1C2, νC5N7, νC4C5 (M1,M2)	1360	1363	3.7
νN1C2, νC5N7, νC4C5 (M1,M2)	1358	1362	3.6
νC2N3, νN1C2 (M1,M2)	1346	1348	2.3
νC2N3, νN1C2 (M1,M2)	1346	1348	1.9
δC8H, νN7C8, δN9H (M1,M2)	1270	1270	-0.2
δC8H, νN7C8, δN9H (M1,M2)	1268	1268	-0.4
δrockNH2, νC5N7, νC2N3 (M1,M2)	1270	1272	2.3
δrockNH2, νC5N7, νC2N3 (M1,M2)	1259	1261	2.1
νC4N9, δr, νC6N6 (M1,M2)	1154	1158	3.6
νC4N9, δr, νC6N6 (M1,M2)	1152	1155	3.4
νC8N9, δN9H (M1,M2)	1087	1082	-5.4
νC8N9, δN9H ((M1,M2)	1087	1081	-5.5
δrockNH2, νN1C6 (M1,M2)	1053	1057	4.6
δrockNH2, νN1C6 (M1,M2)	1046	1050	4.0
γC2H (M1,M2)	977	961	-16.4
γC2H (M1,M2)	977	961	-16.5
δr, νC4C5 (M1,M2)	944	947	2.5
δr, νC4C5 (M1,M2)	944	946	2.5
δ R (M1,M2)	909	912	3.4
δ R (M1,M2)	906	909	3.4
τNH2 (M1,M2)	811	834	23.5
τNH2 (M1,M2)	768	801	33.0
γC8H (M1,M2)	857	837	-20.2

γC8H (M1,M2)	857	837	-20.2
γC8H, τR, τr, γC6N6 (M1,M2)	818	789	-29.4
γC8H, τR, τr, γC6N6 (M1,M2)	814	778	-36.3
νN3C4, νC5N7, νC4N9 (ring breathing)	729	732	3.2
νN3C4, νC5N7, νC4N9 (ring breathing)	727	730	2.8
γC6N6, τr, τR (M1,M2)	691	682	-8.9
γC6N6, τr, τR (M1,M2)	689	680	-8.1
τr (M1,M2)	669	664	-4.9
τr (M1,M2)	667	662	-4.7
δr, νC5C6, δR (M1,M2)	637	641	3.8
δr, νC5C6, δR (M1,M2)	632	634	2.0
γN9H, γC2H, τR, τr (M1,M2)	580	574	-6.3
γN9H, γC2H, τR, τr (M1,M2)	580	574	-6.5
δ R (M1,M2)	543	544	1.5
δ R (M1,M2)	531	532	0.5
γN9H (M1,M2)	527	524	-3.3
γN9H (M1,M2)	527	523	-3.3
δrockNH2, δR, δC6N6 (M1,M2)	534	538	3.5
δrockNH2, δR, δC6N6 (M1,M2)	533	536	3.6
τNH2 (M1,M2)	423	452	28.9
τNH2 (M1,M2)	423	452	28.6
τRr (M1,M2)	298	298	0.2
τRr (M1,M2)	297	296	-0.9
δC6N6, δR, δr (M1,M2)	325	330	4.7
δC6N6, δR, δr (M1,M2)	319	325	6.2
τRr, γwaggNH2 (M1,M2)	223	222	-0.7
τRr, τNH2 (M1,M2)	218	216	-2.8
γwaggNH2, τRr (M1,M2)	161	164	2.7
γwaggNH2, τRr (M1,M2)	160	161	0.5
intermolecular mode	107	110	3.3
intermolecular mode	85	91	5.5
τRr, γC6N6 (M1,M2)	61	48	-12.9
intermolecular mode	40	62	21.8
intermolecular mode	16	20	4.3
intermolecular mode	14	12	-1.3
A-U			
$\nu_{asym}NH_2$ (A)	3694	3693	-1.6
νN9H (A)	3657	3656	-1.2
νN1H (U)	3646	3645	-0.5
$\nu_{sym}NH_2$ (A)	3408	3387	-21.4
νC5H (U)	3266	3259	-7.0
νC8H (A)	3264	3256	-8.0
νC6H (U)	3223	3216	-7.1
νC2H (A)	3195	3189	-6.8
νN3H (U)	2940	2880	-60.6
νC2=O (U)	1788	1803	14.9
νC4=O, ν ring, δN3H (U)	1731	1744	12.6
δscissNH2, νC5C6, νC6N6 (A)	1692	1692	-0.1
νC5=C6 (U)	1668	1669	1.2
νC5C6, νC6N6, δscissNH2 (A)	1644	1644	-0.6
νN3C4, δscissNH2, δN9H (A)	1622	1626	4.1
δN3H (U)	1552	1569	17.1
δC2H, νC8N9, δC8H, νC6N6, δscissNH2 (A), δN3H (U)	1524	1527	2.2
A-ThioU			
$\nu_{asym}NH_2$ (A)	3696	3693	-2.5
νN9H (A)	3657	3656	-1.2
νN1H (ThioU)	3640	3641	0.9
$\nu_{sym}NH_2$ (A)	3436	3409	-27.0
νC5H (ThioU)	3266	3264	-2.7
νC8H (A)	3264	3255	-8.1
νC6H (ThioU)	3226	3222	-3.9
νC2H (A)	3220	3215	-4.7

νN3H (ThioU)	2982	2937	-45.1
νC2=O (ThioU)	1787	1805	18.0
δscissNH2, νC5C6, νC6N6 (A)	1684	1684	0.2
νC5=C6, δNH (ThioU), δscissNH2 (A)	1668	1668	-0.5
δscissNH2, νC5C6 (A)	1639	1639	0.4
νN3C4, δscissNH2, δN9H (A), δN3H (ThioU)	1624	1627	2.8
δN3H (ThioU)	1589	1603	13.5
δC2H, νC8N9, δC8H, νC6N6, δscissNH2 (A), δN3H (ThioU)	1522	1525	2.3
A-T			
$\nu_{asym}NH_2$ (A)	3695	3693	-1.4
νN9H (A)	3658	3656	-1.3
νN1H (T)	3647	3647	0.2
$\nu_{sym}NH_2$ (A)	3406	3385	-21.6
νC8H (A)	3263	3255	-7.9
νC6H (T)	3212	3207	-5.6
νC2H (A)	3195	3188	-6.8
νasymCH3 (T)	3136	3120	-15.8
νasymCH3 (T)	3116	3099	-17.3
νsymCH3 (T)	3056	3040	-16.5
νN3H (T)	2954	2895	-59.0
νC2=O (T)	1786	1800	14.7
νC4=O, δN3H (T)	1719	1731	12.0
νC5=C6, δN3H (T), δscissNH2 (A)	1694	1697	2.5
δscissNH2, νC5C6, νC6N6 (A)	1692	1692	0.0
νC5C6, νC6N6, δscissNH2 (A)	1644	1644	-0.2
νN3C4, δscissNH2, δN9H (A)	1622	1626	4.0
δN3H (T)	1547	1564	17.3
δC2H, νC8N9, δC8H, νC6N6, δscissNH2 (A), δN3H (T)	1524	1526	2.0
G-C			
$\nu_{asym}NH_2$ (G)	3704	3706	2.4
$\nu_{asym}NH_2$ (C)	3689	3686	-3.9
νN9H (G)	3659	3657	-1.9
νN1H (C)	3631	3631	-0.1
$\nu_{sym}NH_2$ (G)	3398	3378	-20.1
νC8H (G)	3263	3254	-9.1
νsymCH (C)	3245	3236	-8.7
νasymCH (C)	3223	3216	-7.3
νN1H, νNH2 (G), νNH2 (C)	3206	3172	-33.8
νNH2 (C), νN1H (G)	3133	3091	-42.4
δN1H , νC6=O (G), δscissNH2, νC2=O (C)	1751	1761	10.6
δscissNH2 (C)	1722	1714	-7.8
δscissNH2 (C), δscissNH2 (G)	1710	1728	17.9
δscissNH2 (G)	1692	1692	-0.2
νC5=C6, δscissNH2 (C), δscissNH2 (G)	1674	1672	-1.8
δN1H, δscissNH2 (G)	1655	1659	4.3
δN9H, νN3C4 (G)	1614	1620	6.0

a Abbreviations: ν = stretching; δ = in-plane bending; γ = out-of-plane bending; τ = torsional; asym = asymmetric; sym = symmetric; M1 = Monomer 1; M2= Monomer 2.

Table. Harmonic vibrational frequencies for uracil and 2-thiouracil molecules, computed at B3LYP-D3/N07D level of theory compared with B2PLYP-D3/maug-cc-pVTZ.

Mode	B2PLYP-D3/maug-cc-pVTZ	B3LYP-D3/N07D		corrected B3LYP-D3/N07D	
Assignment a	harm	harm	Δharm	harm	Δharm
Uracil					
νN1H	3648	3647	-0.9	3655	6.7
νN3H	3601	3607	6.3	3620	19.3
νC2=O	1793	1810	17.0	1792	-1.3
νC4=O	1758	1776	18.1	1761	3.1
2-Thiouracil					
νN1H	3631	3634	3.0	3643	12.5
νN3H	3588	3599	10.6	3613	24.8
νC4=O	1761	1783	21.9	1768	6.2

a Abbreviations: ν = stretching; δ = in-plane bending; γ = out-of-plane bending; τ = torsional; sciss = scissoring; asym = asymmetric; sym = symmetric; M1 = Monomer 1; M2 = Monomer 2.