Supporting Information

Is Non-Statistical Dissociation a General Feature of Guanine–Cytosine Base-Pair ions? Collision-Induced Dissociation of Protonated 9-Methylguanine–1-Methylcytosine Watson-Crick Base Pair, and Comparison with Its Deprotonated and Radical Cation Analogues

Yan Sun,[ab] May Myat Moe[ab] and Jianbo Liu*[ab]
[a] Department of Chemistry and Biochemistry, Queens College of the City University of New York, 65-30 Kissena Blvd., Queens, NY 11367, USA; [b] Ph.D. Program in Chemistry, The Graduate Center of the City University of New York, 365 5th Ave., New York, NY 10016, USA

Table of Contents

*Corresponding author. E-mail: jianbo.liu@qc.cuny.edu. Telephone: 1-718-997-3271.

Cartesian coordinates for the structures in Figure 1, optimized at ωB97XD/6-311++ G(d,p).

WC-[9MG·1MC + H]$^+$_1

C1	-1.344607	1.139656	-0.007738
C2	-2.750646	0.868351	-0.006000
H3	0.419252	0.070300	-0.003946
C4	-1.167315	-1.311883	0.002279
C5	-4.945169	0.927111	-0.007283
N6	-0.623553	-0.045204	-0.003646
N7	-3.859422	1.687482	-0.010892
N8	-4.588053	-0.362581	-0.000684
N9	-2.482443	-1.544398	0.006206
C10	-3.200802	-0.431519	0.001116
N11	-0.321069	-2.329237	0.004555
H12	-0.715312	-3.254924	0.008564
H13	0.703108	-2.197367	-0.002227
O14	-0.821902	2.242497	-0.011983
H15	-5.960830	1.288081	-0.010066
C16	2.925698	-0.783832	-0.005736
N17	2.209024	0.368134	-0.000879
C18	2.821505	1.551262	0.008146
C19	4.942760	0.493053	0.008663
N20	4.320193	-0.711153	-0.001461
H21	6.025449	0.470228	0.012033
O22	2.397843	-1.896085	-0.013814
N23	2.064823	2.651688	0.011594
H24	1.049327	2.578124	0.003469
H25	2.490778	3.561352	0.017060
C26	4.247353	1.651397	0.014161
H27	4.752289	2.606212	0.022363
C28	5.066710	-1.967582	-0.009225
H29	4.806131	-2.559777	0.867519
H30	4.820573	-2.540434	-0.902930
H31	6.131923	-1.741732	0.001975
C32	-5.472907	-1.523749	0.019678
H33	-5.195580	-2.191275	-0.794556
H34	-5.360506	-2.044945	0.969597
H35	-6.501130	-1.189344	-0.105547
H36	-3.844982	2.697492	-0.018865

2

C1	-1.284171	1.030301	-0.023543
C2	-2.702395	0.837982	-0.017368
H3	1.153117	0.135215	-0.015906
C4	-1.188188	-1.333872	0.007056
C5	-4.896716	0.985391	-0.011658
N6	-0.568762	-0.123043	-0.011686
N7	-3.779310	1.700049	-0.026624
N8	-4.591717	-0.317983	0.007058
N9	-2.515816	-1.565850	0.018659
C10	-3.206262	-0.440947	0.004847
N11	-0.397520	-2.416685	0.017482
H12	-0.833547	-3.321656	0.021871
H13	0.611200	-2.333519	-0.009436
O14	-0.767129	2.165369	-0.037880
H15	-5.896558	1.387117	-0.015189
C16	2.978902	-0.836284	-0.020115
N17	2.205900	0.307287	-0.007844
C18	2.696300	1.569535	0.019057
C19	4.878337	0.613706	0.032544
N20	4.353652	-0.637933	0.003677
H21	5.959589	0.670778	0.048334
O22	2.497709	-1.946783	-0.049053
N23	1.855379	2.576318	0.023309
H24	0.811726	2.428057	-0.001082
H25	2.221506	3.513962	0.043144
C26	4.112804	1.727664	0.041568
H27	4.559262	2.710164	0.065515
C28	5.195293	-1.837444	-0.017550
H29	4.931579	-2.485877	0.816716
H30	5.043135	-2.380042	-0.950194
H31	6.236395	-1.532080	0.067379
C32	-5.520437	-1.440805	0.043364
H33	-5.271611	-2.129717	-0.762437
H34	-5.426829	-1.956436	0.998595
H35	-6.535612	-1.068675	-0.083694
H36	-3.721445	2.707550	-0.045572

3

C1	1.108760	-0.610134	0.000524
C2	2.464277	-0.896992	0.000183
H3	-0.221181	0.983479	0.000364
C4	1.722927	1.721381	-0.002697
C5	4.407874	-1.701894	-0.002281
N6	0.787000	0.714382	-0.000770
N7	3.167897	-2.080913	-0.000011
N8	4.580445	-0.327431	-0.006016
N9	3.017627	1.503602	-0.002804
C10	3.334886	0.204487	-0.002107
N11	1.239285	2.975550	-0.004319
H12	1.895699	3.736960	-0.003520
H13	0.251468	3.166161	-0.002436
O14	0.169278	-1.498562	0.002210
H15	5.261833	-2.365049	-0.004049
C16	-2.670864	0.586508	0.001184
N17	-2.340711	-0.729570	0.000547
C18	-3.278858	-1.677243	-0.000378
C19	-4.971692	-0.023922	0.000173
N20	-4.013951	0.937586	0.001072
H21	-5.996332	0.325953	0.000097
O22	-1.816314	1.478420	0.001843
N23	-2.882569	-2.953881	-0.001077
H24	-1.902595	-3.189969	-0.000984
H25	-3.551352	-3.704360	-0.001786
C26	-4.662998	-1.340489	-0.000583
H27	-5.435282	-2.095327	-0.001299
C28	-4.348979	2.362786	0.001772
H29	-3.933349	2.839043	0.889006
H30	-3.933793	2.839840	-0.885249

H31	-5.432384	2.466620	0.002093
C32	5.832235	0.412523	0.010207
H33	5.816353	1.175118	-0.767697
H34	5.978753	0.887949	0.980616
H35	6.648354	-0.282313	-0.181661
H36	-0.780478	-1.120312	0.001764

4

C1	1.082246	-0.484570	-0.069112
C2	2.439862	-0.847865	-0.031715
H3	-0.069012	1.225314	-0.062043
C4	1.909275	1.825602	-0.023471
C5	4.318561	-1.800871	0.024789
N6	0.896195	0.896657	-0.061652
N7	3.051141	-2.080909	-0.020510
N8	4.590735	-0.446001	0.042623
N9	3.175373	1.506140	0.009018
C10	3.385191	0.176321	0.008933
N11	1.533209	3.125604	0.013318
H12	2.266180	3.809532	-0.071545
H13	0.597586	3.405033	-0.225990
O14	0.083235	-1.233221	-0.103324
H15	5.119086	-2.526908	0.045395
C16	-2.836490	0.673859	-0.027608
N17	-2.377831	-0.620378	-0.043752
C18	-3.142563	-1.722488	0.003212
C19	-5.020716	-0.280240	0.080426
N20	-4.216502	0.812317	0.038380
H21	-6.083274	-0.077301	0.130586
O22	-2.080667	1.623144	-0.066399
N23	-2.526695	-2.895308	-0.010891
H24	-1.513662	-2.941615	-0.048312
H25	-3.049561	-3.754301	0.023201
C26	-4.549271	-1.552746	0.065157
H27	-5.221925	-2.396198	0.101886
C28	-4.750848	2.178389	0.057932
H29	-4.320542	2.725313	0.895622
H30	-4.496090	2.687408	-0.871070
H31	-5.832087	2.126577	0.167239
C32	5.889859	0.199998	0.112622
H33	5.970830	0.950264	-0.673534
H34	6.023665	0.679621	1.082979
H35	6.661890	-0.555191	-0.027951
H36	-1.303645	-0.756113	-0.081417

5

C1	-1.434885	1.041919	-0.173307
C2	-2.791822	0.867764	-0.123451
H3	0.393558	0.089666	-0.070360
C4	-1.190491	-1.320235	0.077257
C5	-4.885904	0.997544	-0.079826
N6	-0.650116	-0.049742	-0.069130
N7	-3.840927	1.758526	-0.196140
N8	-4.596661	-0.350086	0.066191
N9	-2.499553	-1.542371	0.139908
C10	-3.243132	-0.451583	0.040166
N11	-0.335975	-2.328632	0.161594
H12	-0.729753	-3.250839	0.247345
H13	0.676634	-2.203419	0.017614
O14	-0.819371	2.205876	-0.312914
H15	-5.910289	1.343342	-0.091414
C16	2.888329	-0.772245	-0.104138
N17	2.203283	0.398636	0.009144
C18	2.860248	1.544449	0.173475
C19	4.943295	0.421861	0.116457
N20	4.283065	-0.747207	-0.055935
H21	6.023910	0.360686	0.149536
O22	2.328638	-1.856833	-0.247175
N23	2.144569	2.672524	0.282004
H24	1.143572	2.643584	0.166543
H25	2.599122	3.563245	0.377048
C26	4.283519	1.595389	0.239658
H27	4.815476	2.525338	0.376271
C28	4.988825	-2.021724	-0.188807
H29	4.672090	-2.704148	0.599010
H30	4.761821	-2.473049	-1.154113
H31	6.058865	-1.837551	-0.109359
C32	-5.538030	-1.448986	0.225271
H33	-5.364419	-2.197343	-0.547644
H34	-5.416385	-1.906252	1.207291
H35	-6.548901	-1.056308	0.128739
H36	-1.482952	2.904246	-0.395785

6

C1	-1.375510	1.179667	0.000432
C2	-2.793172	0.928994	-0.003378
H3	0.427119	0.111566	0.005079
C4	-1.090913	-1.283058	0.009111
C5	-4.904089	1.040303	-0.015256
N6	-0.618485	-0.028082	0.004478
N7	-3.851878	1.798729	-0.013111
N8	-4.602488	-0.313765	-0.008658
N9	-2.435662	-1.475072	0.007391
C10	-3.251810	-0.363285	0.000443
N11	-0.261670	-2.306047	0.016101
H12	-0.609526	-3.250365	0.012355
H13	0.779443	-2.147849	0.009923
O14	-0.797161	2.238879	0.000164
H15	-5.930903	1.376538	-0.022523
C16	2.901023	-0.771061	-0.002341
N17	2.189060	0.378768	0.004202
C18	2.808225	1.563806	0.007081
C19	4.921845	0.488365	-0.003520
N20	4.289988	-0.713494	-0.007150
H21	6.004119	0.457258	-0.007194
O22	2.363255	-1.886403	-0.004436
N23	2.060419	2.665067	0.012847
H24	1.043727	2.599686	0.010908
H25	2.490555	3.573383	0.013878
C26	4.234837	1.650489	0.003996
H27	4.746519	2.601746	0.006862
C28	5.030312	-1.974764	-0.016270

H29	4.775621	-2.561298	0.865855
H30	4.774822	-2.549130	-0.906205
H31	6.096274	-1.753298	-0.015321
C32	-5.536842	-1.427630	0.005197
H33	-5.352181	-2.092411	-0.841153
H34	-5.466201	-1.978725	0.945135
H35	-6.545661	-1.029858	-0.088473
H36	-2.810901	-2.410734	0.019365

7

C1	-1.306869	1.042941	-0.006895
C2	-2.740212	0.897539	-0.018916
H3	1.169835	0.178459	-0.003440
C4	-1.149929	-1.329454	0.033003
C5	-4.843664	1.134991	-0.041934
N6	-0.579297	-0.144298	0.011206
N7	-3.749044	1.830152	-0.046474
N8	-4.623818	-0.235397	-0.014746
N9	-2.511055	-1.500938	0.023678
C10	-3.276700	-0.363020	0.002277
N11	-0.394053	-2.436866	0.080564
H12	-0.791205	-3.353849	-0.022394
H13	0.617680	-2.336125	0.028963
O14	-0.719295	2.122068	-0.013869
H15	-5.849050	1.530743	-0.058066
C16	2.962484	-0.819526	-0.025917
N17	2.213810	0.337827	-0.003837
C18	2.724671	1.594347	0.024377
C19	4.886151	0.593947	0.013429
N20	4.337258	-0.649641	-0.015041
H21	5.968353	0.629301	0.018698
O22	2.452862	-1.920584	-0.052644
N23	1.897769	2.609961	0.040718
H24	0.859096	2.460831	0.023350
H25	2.266690	3.546877	0.060652
C26	4.143939	1.723045	0.034099
H27	4.610240	2.696307	0.057537
C28	5.158317	-1.863906	-0.047105
H29	4.890306	-2.510381	0.787243
H30	4.991027	-2.399496	-0.981157
H31	6.204907	-1.576630	0.031511
C32	-5.619615	-1.291195	0.015816
H33	-5.468235	-1.985757	-0.813323
H34	-5.587503	-1.827478	0.966773
H35	-6.604097	-0.839606	-0.093635
H36	-2.919012	-2.418930	0.103497

8

C1	-1.407646	0.960030	-0.224292
C2	-2.780536	0.832519	-0.165808
H3	1.164011	0.176064	-0.085070
C4	-1.192844	-1.304905	0.131399
C5	-4.875474	0.993758	-0.129874
N6	-0.607979	-0.082250	-0.074699
N7	-3.816234	1.734385	-0.281546
N8	-4.605521	-0.344502	0.080797
N9	-2.502238	-1.548351	0.209026
C10	-3.246898	-0.462193	0.059365
N11	-0.358466	-2.352603	0.293843
H12	-0.784688	-3.262507	0.338550
H13	0.609376	-2.285784	0.008558
O14	-0.815512	2.156856	-0.426197
H15	-5.894354	1.354108	-0.159228
C16	2.968182	-0.825893	-0.190426
N17	2.211042	0.324558	-0.029982
C18	2.721478	1.545005	0.235641
C19	4.879887	0.551600	0.205377
N20	4.343366	-0.659641	-0.070055
H21	5.959208	0.582627	0.288448
O22	2.470155	-1.901208	-0.417104
N23	1.897797	2.570062	0.362707
H24	0.899891	2.481739	0.168739
H25	2.271174	3.485022	0.553871
C26	4.128217	1.667683	0.367992
H27	4.586218	2.621857	0.579667
C28	5.167115	-1.862743	-0.236741
H29	4.895157	-2.600458	0.517082
H30	4.999765	-2.287412	-1.225648
H31	6.213039	-1.585171	-0.123621
C32	-5.558219	-1.422889	0.282028
H33	-5.433543	-2.179773	-0.492715
H34	-5.405033	-1.880201	1.259803
H35	-6.565508	-1.012447	0.227614
H36	-1.503800	2.823711	-0.548257

9

C1	1.298400	1.046787	-0.069743
C2	2.656495	0.893217	-0.249729
H3	-0.416435	0.008823	0.465002
C4	1.203630	-1.306048	0.462134
C5	4.729610	1.041249	-0.567839
N6	0.606863	-0.068729	0.291805
N7	3.661185	1.773449	-0.589526
N8	4.505247	-0.284711	-0.227547
N9	2.499365	-1.495553	0.316015
C10	3.171681	-0.396877	-0.023445
N11	0.396496	-2.313695	0.807313
H12	0.823701	-3.222597	0.876074
H13	-0.616691	-2.254982	0.689640
O14	0.689178	2.192198	-0.233653
H15	5.729153	1.393194	-0.782971
C16	-2.869944	-0.866775	0.108892
N17	-2.210450	0.237946	0.571168
C18	-2.743114	1.437157	0.463396
C19	-4.655790	0.561202	-0.588781
N20	-4.137875	-0.675830	-0.459072
H21	-5.631784	0.626012	-1.053834
O22	-2.391602	-1.987937	0.159348
N23	-1.960945	2.474577	0.943419
H24	-0.251276	2.214136	0.032787
H25	-2.391294	3.389303	0.944403
C26	-3.993686	1.667231	-0.148659

H27	-4.427021	2.651861	-0.242740
C28	-4.842512	-1.867709	-0.937741
H29	-4.277789	-2.329688	-1.747133
H30	-4.936728	-2.584691	-0.123573
H31	-5.828940	-1.573965	-1.291838
C32	5.486594	-1.356040	-0.149706
H33	5.145367	-2.090475	0.578032
H34	5.605647	-1.837745	-1.121183
H35	6.440066	-0.941846	0.175388
H36	-1.513953	2.266024	1.828699

10

C1	1.420740	1.244786	-0.352912
C2	2.774911	0.939852	-0.013424
H3	-0.295299	0.181474	-0.748768
C4	1.206818	-1.194197	-0.592378
C5	4.792559	0.930866	0.598280
N6	0.716114	0.068466	-0.667719
N7	3.812259	1.753538	0.354686
N8	4.461324	-0.392588	0.419679
N9	2.414292	-1.498967	-0.259194
C10	3.161004	-0.395804	0.026581
N11	0.246684	-2.199542	-0.891595
H12	0.639389	-3.101158	-0.634948
H13	0.067160	-2.222585	-1.893707
O14	0.828706	2.316124	-0.379363
H15	5.786503	1.217595	0.911790
C16	-2.857975	-0.740678	0.046455
N17	-2.140330	0.330373	-0.185295
C18	-2.704013	1.555759	-0.074101
C19	-4.784227	0.522687	0.437655
N20	-4.178922	-0.702182	0.366108
H21	-5.838458	0.513232	0.680655
O22	-2.349509	-1.935673	-0.014829
N23	-1.930429	2.606954	-0.245372
H24	-0.904264	2.510012	-0.368220
H25	-2.314325	3.534228	-0.159361
C26	-4.099531	1.664662	0.223472
H27	-4.590807	2.624617	0.293506
C28	-4.915453	-1.947048	0.628133
H29	-4.870993	-2.595137	-0.245769
H30	-4.479587	-2.460601	1.483939
H31	-5.951150	-1.692330	0.841976
C32	5.317452	-1.554028	0.590350
H33	4.860810	-2.254910	1.289106
H34	5.476887	-2.049537	-0.367755
H35	6.274839	-1.222172	0.989182
H36	-1.374932	-1.949836	-0.265839

11

C1	1.380693	0.813105	-0.820388
C2	2.673976	0.782052	-0.347413
H3	-1.088909	0.124662	-0.492424
C4	1.102074	-1.412600	-0.244558
C5	4.679273	1.010396	0.248591
N6	0.590570	-0.253310	-0.749304
N7	3.707797	1.693305	-0.274395
N8	4.367266	-0.307378	0.532693
N9	2.342032	-1.576989	0.213743
C10	3.072307	-0.472810	0.152723
N11	0.256078	-2.462025	-0.181341
H12	0.630410	-3.349274	0.106615
H13	-0.645464	-2.422022	-0.633713
O14	0.832771	1.950104	-1.329147
H15	5.665358	1.400286	0.461418
C16	-2.956484	-0.715006	-0.290721
N17	-2.073784	0.350835	-0.175357
C18	-2.365365	1.536368	0.398102
C19	-4.545762	0.686477	0.813556
N20	-4.229867	-0.489032	0.223001
H21	-5.556748	0.767435	1.193450
O22	-2.637600	-1.760268	-0.798913
N23	-1.438753	2.481062	0.441825
H24	0.330129	1.720943	-2.118414
H25	-1.654616	3.368462	0.866014
C26	-3.667718	1.714097	0.928829
H27	-3.955947	2.641836	1.399371
C28	-5.191632	-1.591426	0.104468
H29	-5.350180	-1.826832	-0.947199
H30	-4.802423	-2.473002	0.611943
H31	-6.129610	-1.283418	0.561691
C32	5.237848	-1.330859	1.084656
H33	4.769144	-1.783425	1.958405
H34	5.431885	-2.103245	0.339557
H35	6.178136	-0.866911	1.379044
H36	-0.547175	2.391773	-0.044415

12

C1	-1.318475	1.178141	0.011537
C2	-2.784903	0.931779	0.004630
H3	0.446050	0.108782	0.014484
C4	-1.149604	-1.267940	0.010751
C5	-4.956725	1.000447	-0.010565
N6	-0.601701	-0.003263	0.014041
N7	-3.738811	1.771516	-0.003363
N8	-4.559234	-0.406069	-0.001573
N9	-2.474242	-1.528768	0.004470
C10	-3.239051	-0.467753	0.002829
N11	-0.314972	-2.275557	0.013046
H12	-0.715889	-3.200872	0.009621
H13	0.720860	-2.145906	0.015159
O14	-0.797920	2.264335	0.013863
H15	-5.554801	1.249578	0.872256
C16	2.908356	-0.783014	0.004257
N17	2.216646	0.382413	0.006506
C18	2.856880	1.553115	-0.001570
C19	4.951325	0.443635	-0.015979
N20	4.300094	-0.746246	-0.007664
H21	6.032974	0.394667	-0.025125
O22	2.351974	-1.885135	0.012119
N23	2.127448	2.670640	0.001388
H24	1.113124	2.623425	0.008951

H25	2.572325	3.571576	-0.004662
C26	4.283660	1.617978	-0.013301
H27	4.811049	2.560573	-0.020133
C28	5.017995	-2.020550	-0.009534
H29	4.763550	-2.591233	0.883060
H30	4.740301	-2.601553	-0.888375
H31	6.087649	-1.818175	-0.024986
C32	-5.481897	-1.526961	-0.023948
H33	-4.908931	-2.444957	0.095483
H34	-6.196889	-1.434237	0.794798
H35	-6.016652	-1.554162	-0.975238
H36	-5.539120	1.242953	-0.905747

13

C1	-1.386047	1.254391	0.187210
C2	-2.773288	0.943618	-0.010851
H3	0.397275	0.202460	0.395600
C4	-1.158443	-1.171509	0.347251
C5	-4.850991	0.946291	-0.368853
N6	-0.636014	0.066997	0.378080
N7	-3.842816	1.763024	-0.233821
N8	-4.507850	-0.379071	-0.251370
N9	-2.387394	-1.491670	0.162812
C10	-3.168999	-0.388284	-0.020063
N11	-0.196450	-2.242434	0.581473
H12	-0.518424	-3.072473	0.083126
H13	0.907344	-1.999307	0.281451
O14	-0.812385	2.326850	0.201470
H15	-5.873719	1.241275	-0.556682
C16	2.802869	-0.751827	-0.021559
N17	2.137967	0.393141	0.144811
C18	2.768823	1.575876	0.072877
C19	4.823789	0.445243	-0.286359
N20	4.161495	-0.745537	-0.243427
H21	5.891086	0.385933	-0.456057
O22	2.224689	-1.871110	0.016399
N23	2.038792	2.674611	0.196945
H24	1.016176	2.616433	0.262250
H25	2.468439	3.581888	0.131684
C26	4.182659	1.623172	-0.132763
H27	4.720252	2.559187	-0.177883
C28	4.855519	-2.022885	-0.426772
H29	4.741758	-2.638773	0.464436
H30	4.436560	-2.551506	-1.281904
H31	5.910749	-1.821864	-0.601160
C32	-5.386561	-1.534336	-0.331144
H33	-5.005965	-2.241659	-1.067736
H34	-5.459184	-2.023385	0.640754
H35	-6.374854	-1.195724	-0.638089
H36	-0.186025	-2.480335	1.574895

14

C1	-1.367995	1.108653	0.286910
C2	-2.799653	0.817977	0.690618
H3	0.428328	0.088620	0.104501
C4	-1.138755	-1.316964	0.149330
C5	-4.797681	1.007316	-0.093648
N6	-0.613048	-0.052219	0.210375
N7	-3.865302	1.737996	0.365383
N8	-4.491955	-0.368531	-0.222479
N9	-2.465384	-1.563776	0.006426
C10	-3.215836	-0.513897	0.147346
N11	-0.306031	-2.324100	0.153614
H12	-0.698142	-3.247644	0.051154
H13	0.727245	-2.184161	0.207206
O14	-0.894667	2.201353	0.134986
H15	-5.776684	1.361899	-0.393771
C16	2.880234	-0.755528	0.057127
N17	2.160507	0.388991	-0.035776
C18	2.766381	1.564701	-0.212082
C19	4.884626	0.502022	-0.222478
N20	4.267488	-0.691659	-0.036290
H21	5.964955	0.474265	-0.289671
O22	2.352497	-1.859659	0.221817
N23	2.007038	2.659659	-0.287462
H24	0.999094	2.595993	-0.182566
H25	2.425946	3.564980	-0.408454
C26	4.187395	1.655454	-0.318273
H27	4.688812	2.600745	-0.465261
C28	5.018610	-1.942076	0.071766
H29	4.842277	-2.398986	1.045128
H30	4.696513	-2.635846	-0.703859
H31	6.078609	-1.723955	-0.046651
C32	-5.336981	-1.383857	-0.836991
H33	-5.465352	-1.175166	-1.900123
H34	-4.849988	-2.349420	-0.714051
H35	-6.307126	-1.399487	-0.341028
H36	-2.752405	0.727276	1.788726

15

C1	1.257693	1.058243	-0.018652
C2	2.739749	0.904174	-0.008453
H3	-1.181064	0.176658	-0.016742
C4	1.190276	-1.298630	-0.013736
C5	4.910245	1.072513	0.012645
N6	0.556609	-0.099606	-0.020390
N7	3.656158	1.787098	0.000322
N8	4.579850	-0.349757	0.005287
N9	2.533101	-1.551085	-0.002968
C10	3.259680	-0.470159	-0.002076
N11	0.421915	-2.377506	-0.016722
H12	0.869291	-3.279218	-0.010850
H13	-0.592071	-2.301536	-0.022966
O14	0.732576	2.166203	-0.023451
H15	5.498994	1.347792	-0.868708
C16	-2.970989	-0.836591	-0.005752
N17	-2.230837	0.328295	-0.007603
C18	-2.754189	1.577374	0.003297
C19	-4.906771	0.560467	0.024235
N20	-4.348259	-0.677143	0.012628
H21	-5.989197	0.587692	0.037429
O22	-2.453574	-1.932464	-0.018881

N23	-1.939066	2.606687	-0.001863
H24	-0.904828	2.480357	-0.013191
H25	-2.320893	3.538393	0.006507
C26	-4.172817	1.696370	0.020213
H27	-4.646777	2.666138	0.030295
C28	-5.157438	-1.900232	0.010978
H29	-4.964818	-2.468316	-0.898449
H30	-4.899950	-2.512208	0.874397
H31	-6.208080	-1.620812	0.057054
C32	5.548433	-1.427656	0.035471
H33	5.013735	-2.369708	-0.076610
H34	6.259927	-1.314558	-0.784349
H35	6.086054	-1.428461	0.986038
H36	5.478117	1.343764	0.908947

16

C1	1.307985	0.994918	-0.286369
C2	2.757113	0.784704	-0.694021
H3	-1.131521	0.162870	-0.060722
C4	1.176232	-1.344862	-0.144714
C5	4.754827	1.070746	0.069421
N6	0.569204	-0.143368	-0.192506
N7	3.788519	1.755780	-0.392380
N8	4.513274	-0.312045	0.219282
N9	2.519015	-1.578035	0.033917
C10	3.234901	-0.515678	-0.136735
N11	0.414213	-2.426012	-0.184003
H12	0.854921	-3.325397	-0.082863
H13	-0.597469	-2.347892	-0.254601
O14	0.832562	2.110598	-0.151899
H15	5.720379	1.472173	0.354139
C16	-2.945859	-0.807101	-0.064298
N17	-2.177059	0.335746	0.018797
C18	-2.663719	1.585139	0.202880
C19	-4.837274	0.616134	0.244030
N20	-4.315145	-0.622725	0.053710
H21	-5.915750	0.664101	0.328224
O22	-2.457987	-1.904405	-0.229137
N23	-1.821273	2.592076	0.258378
H24	-0.798632	2.452276	0.133913
H25	-2.175225	3.525474	0.390370
C26	-4.074245	1.730241	0.325573
H27	-4.521117	2.701336	0.475466
C28	-5.156451	-1.820577	-0.036165
H29	-5.025319	-2.290966	-1.010001
H30	-4.872471	-2.528487	0.741298
H31	-6.195430	-1.525201	0.095073
C32	5.395196	-1.279370	0.853665
H33	5.499202	-1.061965	1.918162
H34	4.955159	-2.267470	0.730628
H35	6.373216	-1.254891	0.373284
H36	2.705989	0.678819	-1.790060

17

C1	-1.284681	1.089243	0.162661
C2	-2.695579	0.909362	0.008864
H3	1.090821	0.228342	0.177920
C4	-1.225494	-1.243737	0.240462
C5	-4.782044	1.090962	-0.258155
N6	-0.567242	-0.101668	0.282332
N7	-3.709020	1.820323	-0.144577
N8	-4.543755	-0.263567	-0.192794
N9	-2.483689	-1.530216	0.098780
C10	-3.200156	-0.384223	-0.019139
N11	-0.360535	-2.441523	0.411452
H12	-0.708876	-3.190072	-0.188440
H13	-0.414408	-2.772169	1.376044
O14	-0.689006	2.174969	0.187320
H15	-5.784634	1.471925	-0.394477
C16	2.849186	-0.795114	-0.041200
N17	2.142637	0.369993	0.069472
C18	2.685531	1.617423	0.053739
C19	4.803620	0.552934	-0.192719
N20	4.213441	-0.678027	-0.180680
H21	5.880512	0.552860	-0.303209
O22	2.298740	-1.890410	-0.017134
N23	1.884210	2.642221	0.157911
H24	0.829589	2.498280	0.205597
H25	2.268743	3.573607	0.141283
C26	4.104764	1.701737	-0.079648
H27	4.601689	2.660086	-0.097530
C28	4.992561	-1.915425	-0.297032
H29	4.895330	-2.502320	0.615768
H30	4.629430	-2.500562	-1.140570
H31	6.036481	-1.653175	-0.455591
C32	-5.512710	-1.341730	-0.267122
H33	-5.207285	-2.065142	-1.023190
H34	-5.602412	-1.842170	0.698056
H35	-6.478453	-0.921549	-0.544281
H36	0.643270	-2.225750	0.193590

18

C1	-1.433273	1.012717	0.155480
C2	-2.843895	0.896570	0.082015
H3	0.207009	-0.218718	0.126103
C4	-1.456308	-1.447149	-0.002432
C5	-4.931468	1.173931	-0.025831
N6	-0.809604	-0.242954	0.106574
N7	-3.829746	1.854202	0.084386
N8	-4.735270	-0.190157	-0.106906
N9	-2.750512	-1.566987	-0.071792
C10	-3.391429	-0.376462	-0.035296
N11	-0.658695	-2.553793	-0.083336
H12	-1.149965	-3.428618	0.008713
H13	0.259006	-2.516545	0.329586
O14	-0.741308	2.029334	0.245620
H15	-5.926354	1.595070	-0.060603
C16	3.174179	-0.700065	0.107057
N17	2.307538	0.261887	0.116083
C18	2.732591	1.544325	-0.044731
C19	4.973257	0.753581	-0.235868
N20	4.515105	-0.533750	-0.062542

H21	6.040984	0.859157	-0.372434
O22	2.692978	-1.922053	0.285353
N23	1.835262	2.491627	-0.022214
H24	0.807776	2.272212	0.105855
H25	2.115669	3.452627	-0.142242
C26	4.133673	1.802276	-0.233044
H27	4.508821	2.806786	-0.369928
C28	5.446349	-1.667362	-0.049105
H29	5.415656	-2.178344	0.915830
H30	5.226157	-2.358063	-0.866754
H31	6.454957	-1.288757	-0.196379
C32	-5.744430	-1.228526	-0.208443
H33	-5.432363	-1.967221	-0.945940
H34	-5.887512	-1.720626	0.754864
H35	-6.682271	-0.775380	-0.527096
H36	3.355046	-2.615352	0.212055

19

C1	1.411352	1.034425	-0.033701
C2	2.818648	0.902127	-0.024510
H3	-0.246200	-0.168316	-0.012494
C4	1.399102	-1.426783	0.036848
C5	4.913373	1.144832	-0.015337
N6	0.772038	-0.207111	-0.002307
N7	3.819983	1.845222	-0.043108
N8	4.699006	-0.219257	0.024198
N9	2.697619	-1.565564	0.043124
C10	3.350517	-0.384787	0.016114
N11	0.592658	-2.515500	0.104164
H12	1.042644	-3.409589	0.005909
H13	-0.391341	-2.453245	-0.107382
O14	0.730210	2.070592	-0.063414
H15	5.915912	1.549104	-0.017838
C16	-2.974973	-0.822321	-0.098356
N17	-2.199468	0.255101	-0.084497
C18	-2.666107	1.493597	0.007452
C19	-4.985292	0.569704	0.089302
N20	-4.490601	-0.604278	0.019807
H21	-6.065137	0.674044	0.169667
O22	-2.651779	-1.971179	-0.185434
N23	-1.823158	2.483129	0.044346
H24	-0.760826	2.288922	-0.003623
H25	-2.149530	3.435749	0.109571
C26	-4.145291	1.785771	0.059103
H27	-4.447099	2.381290	-0.812338
C28	-5.309243	-1.823448	0.039915
H29	-5.142889	-2.367496	-0.888259
H30	-4.987202	-2.445325	0.873294
H31	-6.357286	-1.548510	0.145229
C32	5.693796	-1.275634	0.041159
H33	5.452002	-1.995236	0.822991
H34	5.723911	-1.788605	-0.921273
H35	6.668044	-0.833575	0.245726
H36	-4.394282	2.398392	0.933578

20

C1	-1.285987	1.199781	0.116959
C2	-2.760840	0.965659	0.011135
H3	0.429735	0.088301	0.169892
C4	-1.248158	-1.241857	0.114012
C5	-4.752257	0.837014	-0.678862
N6	-0.617966	0.016038	0.200014
N7	-3.599449	1.608999	-0.723659
N8	-4.641335	-0.262540	-0.009861
N9	-2.533105	-1.436550	0.237481
C10	-3.293877	-0.293723	0.595177
N11	-0.418723	-2.256137	-0.096298
H12	-0.814127	-3.181517	-0.094760
H13	0.604009	-2.133500	-0.151170
O14	-0.778977	2.296296	0.114666
H15	-5.660815	1.132065	-1.190390
C16	2.884643	-0.804056	-0.068626
N17	2.213248	0.370033	0.046556
C18	2.871383	1.526558	0.107020
C19	4.948612	0.394118	-0.032934
N20	4.280053	-0.783000	-0.102361
H21	6.029114	0.331488	-0.068488
O22	2.312571	-1.891161	-0.144130
N23	2.159278	2.653229	0.204476
H24	1.144719	2.621049	0.190218
H25	2.617948	3.546427	0.235458
C26	4.298886	1.574262	0.071273
H27	4.839757	2.507748	0.123509
C28	4.976863	-2.062176	-0.223937
H29	4.694806	-2.717054	0.599680
H30	4.707289	-2.546243	-1.162356
H31	6.049941	-1.879149	-0.198393
C32	-5.612476	-1.329428	0.176825
H33	-5.141137	-2.262337	-0.134876
H34	-5.881575	-1.391313	1.231859
H35	-6.496988	-1.124486	-0.423370
H36	-3.446194	-0.199979	1.686226

21

C1	-1.228956	1.104781	0.127455
C2	-2.710580	0.944521	-0.007925
H3	1.155246	0.163703	0.088533
C4	-1.280256	-1.252200	0.147444
C5	-4.684971	0.849465	-0.753664
N6	-0.570475	-0.051667	0.167222
N7	-3.512364	1.581583	-0.796960
N8	-4.634906	-0.220411	-0.029234
N9	-2.566744	-1.442863	0.331325
C10	-3.304383	-0.266367	0.613535
N11	-0.512416	-2.330887	-0.065287
H12	-0.944289	-3.237346	-0.019281
H13	0.494475	-2.251413	-0.137439
O14	-0.724087	2.229517	0.161616
H15	-5.568340	1.145952	-1.307166
C16	2.935258	-0.862846	-0.086439
N17	2.209683	0.304866	0.044301

C18	2.749004	1.543454	0.128593
C19	4.889137	0.511365	-0.029103
N20	4.315949	-0.715594	-0.116779
H21	5.971289	0.528739	-0.064895
O22	2.407055	-1.948665	-0.169367
N23	1.949780	2.580070	0.237151
H24	0.910160	2.475725	0.229156
H25	2.349140	3.502490	0.294719
C26	4.168914	1.649369	0.092597
H27	4.653475	2.611635	0.158689
C28	5.108872	-1.940393	-0.256170
H29	4.854802	-2.634228	0.543811
H30	4.897447	-2.412827	-1.215060
H31	6.163694	-1.679498	-0.196825
C32	-5.644840	-1.244475	0.175326
H33	-5.176261	-2.210578	-0.016587
H34	-5.998179	-1.207750	1.206679
H35	-6.474917	-1.078501	-0.509110
H36	-3.484229	-0.118640	1.694715

22

C1	-1.260639	1.205381	-0.018194
C2	-2.727757	0.955722	-0.026809
H3	0.471094	0.149481	0.092173
C4	-1.087923	-1.310970	0.231142
C5	-4.842654	0.978069	-0.084204
N6	-0.581759	0.047305	0.114879
N7	-3.723769	1.777512	-0.148280
N8	-4.605925	-0.301283	0.078930
N9	-2.525297	-1.479318	0.226760
C10	-3.191922	-0.419621	0.121370
N11	-0.555655	-2.116061	-0.837031
H12	-0.889447	-3.069419	-0.741146
H13	0.464365	-2.128272	-0.737125
O14	-0.777377	2.314481	-0.114295
H15	-5.845261	1.380543	-0.164903
C16	2.818971	-0.792260	0.037959
N17	2.183186	0.407526	0.025676
C18	2.862801	1.551328	0.012963
C19	4.911526	0.360377	0.051156
N20	4.216711	-0.804156	0.056979
H21	5.990720	0.270438	0.064351
O22	2.210303	-1.859582	0.035674
N23	2.167901	2.692415	-0.010914
H24	1.152174	2.669455	-0.054127
H25	2.639453	3.578962	-0.036865
C26	4.291744	1.561596	0.028723
H27	4.856849	2.482127	0.022694
C28	4.884462	-2.103582	0.066235
H29	4.556764	-2.682191	0.929220
H30	4.635627	-2.656824	-0.839344
H31	5.960403	-1.943894	0.117034
C32	-5.550392	-1.412067	0.177004
H33	-5.332068	-2.130669	-0.611846
H34	-5.438535	-1.888470	1.150163
H35	-6.560065	-1.022591	0.062298
H36	-0.802537	-1.659292	1.243323

23

C1	1.244302	1.080974	-0.113894
C2	2.707774	0.914852	-0.013561
H3	-1.163435	0.174091	-0.132072
C4	1.189258	-1.351949	-0.342650
C5	4.808625	1.054539	0.177636
N6	0.581568	-0.065304	-0.222348
N7	3.666350	1.794653	0.139643
N8	4.642719	-0.248033	0.046520
N9	2.626380	-1.524396	-0.191091
C10	3.248142	-0.432333	-0.076779
N11	0.549039	-2.282855	0.551157
H12	0.907434	-3.218629	0.400446
H13	-0.453936	-2.282300	0.382116
O14	0.732043	2.209273	-0.062676
H15	5.787591	1.499483	0.307847
C16	-2.944183	-0.847599	-0.054221
N17	-2.207662	0.321506	-0.061247
C18	-2.726908	1.570525	0.008204
C19	-4.877497	0.550188	0.103680
N20	-4.321607	-0.686513	0.035277
H21	-5.958005	0.576668	0.170463
O22	-2.426670	-1.938421	-0.121813
N23	-1.911466	2.598170	-0.006090
H24	-0.867927	2.474836	-0.045433
H25	-2.295923	3.527123	0.049678
C26	-4.144685	1.686649	0.093003
H27	-4.617569	2.655159	0.151877
C28	-5.130213	-1.908512	0.041677
H29	-4.999913	-2.443289	-0.898714
H30	-4.816053	-2.552623	0.861870
H31	-6.175327	-1.633050	0.168745
C32	5.641357	-1.310802	0.054662
H33	5.417873	-2.004635	0.864111
H34	5.611400	-1.838405	-0.897956
H35	6.623732	-0.866546	0.203991
H36	1.083993	-1.624487	-1.420351

24

C1	-1.382751	1.073015	0.081998
C2	-2.793006	0.913542	0.020855
H3	0.294998	-0.098696	0.143983
C4	-1.324244	-1.389056	0.061987
C5	-4.888619	1.106571	-0.067321
N6	-0.724769	-0.159851	0.103083
N7	-3.803274	1.830368	-0.014443
N8	-4.655469	-0.250072	-0.067281
N9	-2.634666	-1.552011	0.002143
C10	-3.303192	-0.395928	-0.012286
N11	-0.518699	-2.459316	0.085679
H12	-0.950994	-3.366332	0.042859
H13	0.493021	-2.374918	0.100671
O14	-0.728664	2.117310	0.115996
H15	-5.895212	1.498913	-0.106966

C16	2.943697	-0.817821	0.051863
N17	2.186937	0.339260	0.109075
C18	2.690725	1.561730	0.006538
C19	4.950899	0.553089	-0.138757
N20	4.319382	-0.703850	-0.009475
H21	5.550658	0.621309	-1.074748
O22	2.408668	-1.908830	0.067740
N23	1.890640	2.620689	0.034749
H24	0.855358	2.467318	0.093340
H25	2.256472	3.554699	-0.049381
C26	4.104134	1.713987	-0.121634
H27	4.569764	2.691570	-0.205497
C28	5.119807	-1.922883	-0.076395
H29	4.777258	-2.619985	0.686943
H30	5.014965	-2.398294	-1.054141
H31	6.166169	-1.673232	0.100857
C32	-5.631706	-1.323311	-0.142529
H33	-5.573825	-1.820523	-1.111491
H34	-5.440279	-2.049857	0.646729
H35	-6.625830	-0.898859	-0.010070
H36	5.732421	0.704921	0.636396

25

C1	1.374553	1.136073	0.056612
C2	2.834254	0.938258	-0.001389
H3	-1.189344	0.267739	0.131297
C4	1.207184	-1.215028	0.068931
C5	4.944102	0.978056	-0.083981
N6	0.649409	-0.018732	0.092045
N7	3.843762	1.774565	-0.048051
N8	4.694413	-0.329083	-0.063191
N9	2.598052	-1.500034	0.023438
C10	3.301274	-0.437900	-0.006978
N11	0.453865	-2.294981	0.085195
H12	0.896934	-3.200228	0.064765
H13	-0.582850	-2.197459	0.096924
O14	0.866948	2.245690	0.072914
H15	5.952265	1.370274	-0.128819
C16	-2.888010	-0.847044	0.039298
N17	-2.212580	0.353956	0.105294
C18	-2.808989	1.590440	0.012333
C19	-5.005174	0.437501	-0.067642
N20	-4.230811	-0.796847	-0.052021
H21	-5.677218	0.442681	0.805924
O22	-2.246788	-1.901459	0.066027
N23	-1.979367	2.653901	0.027420
H24	-0.966859	2.549218	0.062764
H25	-2.364456	3.579533	-0.038572
C26	-4.168005	1.662936	-0.081063
H27	-4.661811	2.622033	-0.153821
C28	-5.002360	-2.027126	-0.115180
H29	-4.329893	-2.875216	-0.022030
H30	-5.730890	-2.048604	0.699806
H31	-5.533969	-2.088263	-1.068938
C32	5.638708	-1.442513	-0.079292
H33	5.578387	-1.981902	0.865462
H34	5.388597	-2.110838	-0.902145
H35	6.642456	-1.044813	-0.216875
H36	-5.665049	0.420863	-0.948050

Cartesian coordinates for the structures in Figure 2, optimized at ωB97XD/6-311++ G(d,p).

WC-[9MG·1MC + H]$^+$·H_2O_1

C1	-1.264446	0.787026	-0.051738
C2	-2.638948	0.400939	-0.024158
H3	0.589331	-0.115616	-0.053136
C4	-0.864128	-1.633641	-0.013735
C5	-4.818807	0.264528	0.026696
N6	-0.438224	-0.320673	-0.045572
N7	-3.816305	1.119913	-0.015200
N8	-4.350172	-0.994431	0.044707
N9	-2.149912	-1.980663	0.021099
C10	-2.967005	-0.937176	0.014708
N11	0.071012	-2.570807	-0.016936
H12	-0.240687	-3.527205	0.004216
H13	1.079050	-2.352801	-0.060088
O14	-0.817375	1.934623	-0.075846
H15	-5.863974	0.527889	0.043545
C16	3.177531	-0.784228	-0.049199
N17	2.370112	0.306482	-0.022705
C18	2.886278	1.531388	0.053689
C19	5.084234	0.646250	0.085575
N20	4.561176	-0.601162	0.005186
H21	6.164496	0.710195	0.126309
O22	2.742831	-1.933260	-0.117779
N23	2.041090	2.566932	0.073353
H24	1.037728	2.407292	0.020024
H25	2.390238	3.506820	0.131020
C26	4.297419	1.744904	0.113647
H27	4.724375	2.734925	0.178946
C28	5.405600	-1.793766	-0.031789
H29	5.141970	-2.459064	0.789502
H30	5.257363	-2.324765	-0.971881
H31	6.446797	-1.488448	0.059920
C32	-5.129337	-2.226138	0.107756
H33	-4.798560	-2.894719	-0.685442
H34	-4.974327	-2.706306	1.073390
H35	-6.182938	-1.986978	-0.024951
H36	-3.843692	2.157255	-0.043767
O37	-3.021153	3.652617	-0.029886
H38	-2.090994	3.375866	-0.078346
H39	-3.102384	4.524165	-0.417397

2

C1	-0.887644	1.049269	0.000045
C2	-2.281360	0.728722	0.001249
H3	0.912458	0.042280	0.000131
C4	-0.621295	-1.394636	0.003320
C5	-4.480805	0.707643	0.001473
N6	-0.123773	-0.109638	0.001019
N7	-3.421810	1.506557	-0.000189
N8	-4.071800	-0.566740	0.004070
N9	-1.925204	-1.673827	0.005369
C10	-2.684508	-0.586207	0.003976
N11	0.262633	-2.381938	0.003596
H12	-0.098627	-3.320731	0.004778
H13	1.280092	-2.214105	-0.000092
O14	-0.399651	2.169336	-0.001619
H15	-5.523083	1.005820	-0.000027
C16	3.458290	-0.720440	-0.003656
N17	2.698893	0.403649	-0.000514
C18	3.265165	1.609152	0.002828
C19	5.425698	0.632932	0.000412
N20	4.849738	-0.594241	-0.003336
H21	6.508499	0.652150	0.000547
O22	2.974052	-1.851927	-0.006798
N23	2.465870	2.679070	0.005369
H24	1.453263	2.565209	0.003126
H25	2.856139	3.604549	0.007363
C26	4.686451	1.763944	0.003721
H27	5.155189	2.737075	0.006779
C28	5.643036	-1.821336	-0.007837
H29	5.408359	-2.418225	0.873075
H30	5.414411	-2.408023	-0.897219
H31	6.699166	-1.555802	-0.002693
C32	-4.925649	-1.750932	0.009577
H33	-4.695142	-2.358557	-0.864534
H34	-4.727845	-2.328260	0.911898
H35	-5.964324	-1.425192	-0.014622
H36	-3.445738	2.515630	-0.002817
O37	-7.540297	0.604540	-0.014964
H38	-8.110602	0.694903	-0.781574
H39	-8.121152	0.686770	0.744601

3

C1	-1.456962	1.044353	-0.005116
C2	-2.887396	0.959474	-0.010914
H3	0.154684	-0.250664	0.012083
C4	-1.603634	-1.408703	0.019909
C5	-5.055121	1.307456	-0.026293
N6	-0.897404	-0.225001	0.009939
N7	-3.878155	1.917597	-0.027891
N8	-4.870853	-0.018074	-0.009143
N9	-2.939376	-1.466530	0.018145
C10	-3.504618	-0.269464	0.001740
N11	-0.901237	-2.529244	0.032510
H12	-1.416935	-3.393116	0.038115
H13	0.133995	-2.536968	0.025475
O14	-0.796766	2.070072	-0.011868
H15	-6.014465	1.798372	-0.038162

C16	2.508013	-1.459693	-0.001130
N17	1.955079	-0.222167	0.008066
C18	2.726664	0.868693	0.007545
C19	4.682653	-0.473322	-0.015194
N20	3.896968	-1.582240	-0.017674
H21	5.751332	-0.648117	-0.025772
O22	1.832204	-2.491767	0.003375
N23	2.146345	2.066008	0.015160
H24	1.132664	2.139423	0.012393
H25	2.721898	2.900452	0.014482
C26	4.155340	0.768037	-0.001502
H27	4.773695	1.653910	-0.000557
C28	4.462717	-2.928661	-0.031394
H29	4.173876	-3.466281	0.871725
H30	4.092651	-3.477916	-0.896519
H31	5.547720	-2.849697	-0.082152
C32	-5.901348	-1.051364	0.012464
H33	-5.713609	-1.752945	-0.798792
H34	-5.861327	-1.580053	0.964085
H35	-6.875837	-0.583785	-0.115996
H36	-3.729363	2.916505	-0.042269
O37	4.202505	4.173105	0.021435
H38	4.445487	4.689499	0.792217
H39	4.442566	4.706823	-0.738368

4

C1	1.088557	-1.486682	-0.039003
C2	2.511897	-1.327003	-0.017495
H3	-0.586281	-0.287713	-0.047023
C4	1.095664	0.975936	-0.036566
C5	4.693102	-1.565381	0.048799
N6	0.462163	-0.251129	-0.048403
N7	3.549609	-2.233245	0.019609
N8	4.441339	-0.249668	0.032240
N9	2.436483	1.097966	-0.030231
C10	3.064850	-0.068151	-0.010357
N11	0.337651	2.051358	-0.032038
H12	0.806460	2.955006	-0.000170
H13	-0.691281	1.986614	-0.032665
O14	0.485661	-2.547556	-0.044468
H15	5.675394	-2.007524	0.082889
C16	-3.026054	0.738389	-0.011119
N17	-2.396891	-0.464319	-0.022758
C18	-3.095936	-1.597820	-0.002706
C19	-5.132375	-0.385144	0.047058
N20	-4.422279	0.769211	0.027725
H21	-6.209971	-0.281630	0.076076
O22	-2.417991	1.807488	-0.032321
N23	-2.423460	-2.751980	-0.015938
H24	-1.405823	-2.752249	-0.034633
H25	-2.914948	-3.627720	0.001003
C26	-4.524961	-1.591880	0.032348
H27	-5.098803	-2.506899	0.048463
C28	-5.072606	2.077856	0.041891
H29	-4.731188	2.651872	0.902646
H30	-4.822738	2.627899	-0.865130
H31	-6.150055	1.931350	0.100289
C32	5.420643	0.831390	0.058138
H33	5.391574	1.369391	-0.889075
H34	5.176487	1.509627	0.874920
H35	6.411902	0.409324	0.212700
H36	3.451233	-3.238703	0.026605
O37	2.428662	3.993392	0.072854
H38	2.913120	3.177134	-0.100673
H39	2.785263	4.671227	-0.502113

5

C1	1.861575	-1.142022	-0.007360
C2	3.264364	-0.852337	-0.005938
H3	0.081128	-0.095381	-0.003200
C4	1.652319	1.306428	0.003075
C5	5.459586	-0.883342	-0.007488
N6	1.124815	0.032688	-0.002950
N7	4.383383	-1.657224	-0.011115
N8	5.085844	0.401772	-0.000586
N9	2.965324	1.556391	0.006891
C10	3.697612	0.453192	0.001474
N11	0.793668	2.312317	0.005595
H12	1.177310	3.242417	0.009577
H13	-0.231235	2.167476	-0.001446
O14	1.355412	-2.252508	-0.011620
H15	6.479787	-1.231061	-0.010516
C16	-2.425599	0.744530	-0.006624
N17	-1.696866	-0.400421	-0.000922
C18	-2.301469	-1.588605	0.007827
C19	-4.434185	-0.548028	0.005789
N20	-3.816497	0.659193	-0.004109
H21	-5.519081	-0.524089	0.007778
O22	-1.904910	1.862162	-0.014062
N23	-1.533705	-2.683554	0.012345
H24	-0.519543	-2.602451	0.004478
H25	-1.952982	-3.596067	0.017193
C26	-3.723724	-1.699672	0.012440
H27	-4.219763	-2.659302	0.020361
C28	-4.580856	1.906341	-0.012253
H29	-4.326805	2.499675	0.866060
H30	-4.333360	2.484038	-0.902826
H31	-5.641512	1.659836	-0.006287
C32	5.955169	1.574155	0.019876
H33	5.668880	2.238349	-0.794019
H34	5.836000	2.093882	0.969804
H35	6.987864	1.253824	-0.105578

H36	4.380923	-2.667277	-0.019232
O37	-7.600011	0.170987	0.005150
H38	-8.181487	0.154495	-0.757260
H39	-8.180565	0.164543	0.768411

6

C1	-1.536097	-1.354250	0.065529
C2	-2.923734	-1.002696	0.027980
H3	0.279281	-0.375752	0.079089
C4	-1.217767	1.088163	0.029196
C5	-5.117701	-0.930184	-0.030913
N6	-0.751559	-0.212534	0.065649
N7	-4.080059	-1.754041	0.013474
N8	-4.683590	0.335416	-0.046316
N9	-2.517636	1.393605	-0.013487
C10	-3.294982	0.322874	-0.011125
N11	-0.305316	2.038224	0.038268
H12	-0.574616	3.008777	0.000164
H13	0.697183	1.828056	0.077720
O14	-1.071749	-2.483783	0.092064
H15	-6.153195	-1.228693	-0.050659
C16	2.898643	0.363925	0.049228
N17	2.101195	-0.730671	0.048802
C18	2.626918	-1.953989	-0.019273
C19	4.816211	-1.048123	-0.100798
N20	4.280785	0.196926	-0.030310
H21	5.896055	-1.101355	-0.160330
O22	2.448694	1.511435	0.116651
N23	1.796147	-2.998440	-0.013414
H24	0.787391	-2.862692	0.041256
H25	2.158675	-3.934050	-0.063623
C26	4.040583	-2.153359	-0.097727
H27	4.476376	-3.140064	-0.155154
C28	5.116525	1.395261	-0.027453
H29	4.837455	2.044109	-0.857301
H30	4.984074	1.939118	0.907982
H31	6.158289	1.096605	-0.132352
C32	-5.494890	1.547350	-0.108857
H33	-5.183971	2.218756	0.689883
H34	-5.340958	2.035471	-1.070540
H35	-6.543232	1.281432	0.013915
H36	-4.126866	-2.762649	0.037029
O37	1.518739	4.207335	-0.048344
H38	1.932509	5.024748	0.228188
H39	2.188063	3.519054	0.038381

7

C1	-1.385744	0.879665	-0.089476
C2	-2.786976	0.597102	-0.035711
H3	0.396912	-0.182180	-0.088197
C4	-1.180875	-1.567061	-0.033764
C5	-4.981751	0.631170	0.044891
N6	-0.650012	-0.293607	-0.080840
N7	-3.906155	1.403754	-0.013937
N8	-4.610276	-0.653675	0.061714
N9	-2.494325	-1.811181	0.015759
C10	-3.222856	-0.707665	0.013800
N11	-0.328872	-2.576890	-0.038160
H12	-0.720896	-3.503146	-0.001736
H13	0.699164	-2.450495	-0.086500
O14	-0.873884	1.990532	-0.134820
H15	-6.000924	0.981082	0.074941
C16	2.907075	-1.128691	-0.053711
N17	2.195345	0.023755	-0.028188
C18	2.813206	1.204913	0.068463
C19	4.926553	0.133032	0.122029
N20	4.299230	-1.066067	0.020270
H21	6.007499	0.101332	0.178739
O22	2.376105	-2.238235	-0.139030
N23	2.058233	2.298012	0.085360
H24	1.050622	2.221072	0.004506
H25	2.436777	3.228144	0.143922
C26	4.237994	1.293999	0.151606
H27	4.743156	2.244904	0.234326
C28	5.040419	-2.324657	-0.018287
H29	4.714363	-2.972958	0.794300
H30	4.860354	-2.834791	-0.964448
H31	6.102452	-2.108402	0.087256
C32	-5.479970	-1.824240	0.136636
H33	-5.213980	-2.510211	-0.665910
H34	-5.337553	-2.318190	1.097069
H35	-6.515143	-1.505948	0.027819
H36	-3.908390	2.413162	-0.036122
O37	0.437717	4.652081	-0.004776
H38	0.210287	5.497886	-0.391509
H39	-0.308823	4.069617	-0.172138

Cartesian coordinates for the structures in Figure 5, optimized at ωB97XD/6-311++ G(d,p).

WC-[9MG + H_{N7}]$^+$·1MC

C1	-1.344607	1.139656	-0.007738
C2	-2.750646	0.868351	-0.006000
H3	0.419252	0.070300	-0.003946
C4	-1.167315	-1.311883	0.002279
C5	-4.945169	0.927111	-0.007283
N6	-0.623553	-0.045204	-0.003646
N7	-3.859422	1.687482	-0.010892
N8	-4.588053	-0.362581	-0.000684
N9	-2.482443	-1.544398	0.006206
C10	-3.200802	-0.431519	0.001116
N11	-0.321069	-2.329237	0.004555
H12	-0.715312	-3.254924	0.008564
H13	0.703108	-2.197367	-0.002227
O14	-0.821902	2.242497	-0.011983
H15	-5.960830	1.288081	-0.010066
C16	2.925698	-0.783832	-0.005736
N17	2.209024	0.368134	-0.000879
C18	2.821505	1.551262	0.008146
C19	4.942760	0.493053	0.008663
N20	4.320193	-0.711153	-0.001461
H21	6.025449	0.470228	0.012033
O22	2.397843	-1.896085	-0.013814
N23	2.064823	2.651688	0.011594
H24	1.049327	2.578124	0.003469
H25	2.490778	3.561352	0.017060
C26	4.247353	1.651397	0.014161
H27	4.752289	2.606212	0.022363
C28	5.066710	-1.967582	-0.009225
H29	4.806131	-2.559777	0.867519
H30	4.820573	-2.540434	-0.902930
H31	6.131923	-1.741732	0.001975
C32	-5.472907	-1.523749	0.019678
H33	-5.195580	-2.191275	-0.794556
H34	-5.360506	-2.044945	0.969597
H35	-6.501130	-1.189344	-0.105547
H36	-3.844982	2.697492	-0.018865

[9MG + H_{N7}]$^+$

C1	1.153343	1.398909	0.001821
C2	-0.217647	0.964052	0.000918
H3	2.979880	0.480054	0.002068
C4	1.581215	-1.052193	-0.000718
C5	-2.404039	0.785336	-0.004167
N6	1.991747	0.259404	0.001351
N7	-1.406576	1.659263	-0.001278
N8	-1.909173	-0.457417	-0.004582
N9	0.311520	-1.411744	-0.000968
C10	-0.526602	-0.372927	-0.000586
N11	2.526343	-1.999404	-0.002363
H12	2.230141	-2.961506	-0.003605
H13	3.510672	-1.796241	-0.002883
O14	1.585610	2.520603	0.002807
H15	-3.453410	1.032967	-0.006438
C16	-2.668556	-1.707071	0.006628
H17	-2.322552	-2.336480	-0.811447
H18	-2.506895	-2.217311	0.955168
H19	-3.725139	-1.479773	-0.120954
H20	-1.500888	2.666111	-0.002863

1MC

C1	-0.620802	-0.898779	-0.000251
N2	0.733680	-1.069029	0.001555
C3	1.537000	-0.033499	-0.002267
C4	-0.265958	1.493957	0.000540
N5	-1.110731	0.440475	0.000431
H6	-0.722989	2.476718	0.000534
O7	-1.430811	-1.802087	0.000545
N8	2.870630	-0.282576	-0.029124
H9	3.164403	-1.239741	0.070125
H10	3.538544	0.449797	0.126340
C11	1.076265	1.322999	-0.000995
H12	1.751212	2.166740	-0.008572
C13	-2.555952	0.612478	0.001597
H14	-2.989145	0.139043	-0.880024
H15	-2.987852	0.140913	0.884884
H16	-2.786061	1.678194	0.000573

WC-TS_PT1

C1	1.246049	1.069511	0.169034
C2	2.655919	0.832113	0.144679
H3	-0.840623	0.121378	0.029873
C4	1.088509	-1.300268	-0.137752
C5	4.850265	0.929712	0.134328
N6	0.499061	-0.071811	0.025074
N7	3.751364	1.663366	0.247012
N8	4.514228	-0.354175	-0.043006
N9	2.409075	-1.541635	-0.188307
C10	3.127079	-0.443269	-0.042107
N11	0.281453	-2.353945	-0.273912
H12	0.720099	-3.256908	-0.332653
H13	-0.713783	-2.284628	-0.065022
O14	0.758495	2.198405	0.299353
H15	5.859723	1.304250	0.180591
C16	-2.867242	-0.799105	0.154263
N17	-2.091016	0.324413	0.009926
C18	-2.635645	1.541918	-0.191601
C19	-4.804569	0.565685	-0.150233
N20	-4.249169	-0.649295	0.076569
H21	-5.885605	0.593402	-0.205615
O22	-2.393996	-1.906756	0.342579
N23	-1.841361	2.592802	-0.292127
H24	-0.828942	2.512108	-0.090269
H25	-2.248902	3.503397	-0.419521
C26	-4.052527	1.677197	-0.294205
H27	-4.507875	2.641213	-0.464991
C28	-5.060806	-1.857227	0.234191

H29	-4.794906	-2.584496	-0.531993
H30	-4.882559	-2.299068	1.213932
H31	-6.110279	-1.585314	0.136608
C32	5.416392	-1.487551	-0.211871
H33	5.202587	-2.228668	0.557020
H34	5.256923	-1.931323	-1.193826
H35	6.444353	-1.141279	-0.120308
H36	3.717835	2.662413	0.389752

WC-[9MG + H_{N7} – H_{N1}]·[1MC + $H_{N3'}$]$^+$

C1	-1.284171	1.030301	-0.023542
C2	-2.702395	0.837982	-0.017368
H3	1.153117	0.135215	-0.015906
C4	-1.188188	-1.333872	0.007056
C5	-4.896716	0.985391	-0.011658
N6	-0.568762	-0.123043	-0.011686
N7	-3.779310	1.700049	-0.026624
N8	-4.591717	-0.317983	0.007058
N9	-2.515816	-1.565850	0.018659
C10	-3.206262	-0.440947	0.004847
N11	-0.397520	-2.416685	0.017482
H12	-0.833547	-3.321656	0.021871
H13	0.611200	-2.333519	-0.009436
O14	-0.767129	2.165369	-0.037880
H15	-5.896558	1.387117	-0.015189
C16	2.978902	-0.836285	-0.020114
N17	2.205900	0.307287	-0.007844
C18	2.696300	1.569535	0.019057
C19	4.878337	0.613706	0.032544
N20	4.353652	-0.637933	0.003677
H21	5.959589	0.670778	0.048334
O22	2.497709	-1.946783	-0.049052
N23	1.855379	2.576318	0.023309
H24	0.811726	2.428057	-0.001082
H25	2.221506	3.513962	0.043144
C26	4.112804	1.727664	0.041567
H27	4.559262	2.710164	0.065515
C28	5.195293	-1.837444	-0.017550
H29	4.931579	-2.485877	0.816717
H30	5.043134	-2.380043	-0.950194
H31	6.236395	-1.532080	0.067379
C32	-5.520437	-1.440805	0.043363
H33	-5.271611	-2.129717	-0.762437
H34	-5.426829	-1.956436	0.998595
H35	-6.535612	-1.068675	-0.083695
H36	-3.721445	2.707550	-0.045572

[9MG + H_{N7} – H_{N1}]

C1	1.229612	1.341748	0.000866
C2	-0.165310	0.934591	0.008241
C3	1.617038	-0.978822	0.005505
C4	-2.366357	0.804489	-0.004279
N5	2.078963	0.268913	-0.000730
N6	-1.340365	1.647440	0.004050
N7	-1.891813	-0.452030	-0.008344
N8	0.331612	-1.425603	-0.002244
C9	-0.500994	-0.399221	0.000196
N10	2.561273	-1.964241	0.049952
H11	2.269837	-2.897600	-0.180939
H12	3.506702	-1.686921	-0.149028
O13	1.561356	2.522127	-0.006809
H14	-3.408552	1.073516	-0.007428
C15	-2.663432	-1.681556	0.002514
H16	-2.311685	-2.327048	-0.801639
H17	-2.520638	-2.194636	0.953818
H18	-3.717844	-1.448604	-0.141471
H19	-1.389694	2.655543	0.004108

[1MC + $H_{N3'}$]$^+$

H1	1.019507	-1.948978	-0.000001
C2	-0.694774	-0.868730	0.000007
N3	0.705660	-0.985435	0.000010
C4	1.586903	0.038184	0.000001
C5	-0.294550	1.489488	0.000007
N6	-1.151608	0.448891	0.000013
H7	-0.748775	2.472874	0.000001
O8	-1.407140	-1.826590	-0.000002
N9	2.887658	-0.220781	-0.000010
H10	3.256708	-1.158983	-0.000014
H11	3.553817	0.535194	-0.000023
C12	1.059553	1.346100	0.000003
H13	1.708931	2.208215	0.000002
C14	-2.611547	0.627233	-0.000014
H15	-3.034770	0.159534	-0.887891
H16	-3.034822	0.159367	0.887749
H17	-2.828959	1.693118	0.000079

WC-TS_enol

C1	1.347764	0.894301	0.403415
C2	2.694389	0.622492	0.549305
H3	-0.476872	-0.052994	0.155831
C4	1.166472	-1.463286	0.176452
C5	4.603501	1.124935	-0.186656
N6	0.566901	-0.191012	0.282321
N7	3.499371	1.684021	0.268388
N8	4.497370	-0.244658	-0.237495
N9	2.478177	-1.679955	0.038767
C10	3.213211	-0.571268	0.164941
N11	0.319456	-2.480654	0.171095
H12	0.704333	-3.402721	0.049729
H13	-0.698610	-2.334854	0.198629
O14	1.104996	2.135055	0.243143
H15	5.502229	1.639923	-0.491026
C16	-2.889358	-0.747011	0.023546
N17	-2.132988	0.382264	-0.012687
C18	-2.694635	1.581424	-0.147483
C19	-4.845972	0.592319	-0.235841
N20	-4.274163	-0.627805	-0.091588
H21	-5.925388	0.606075	-0.321322
O22	-2.397627	-1.866140	0.153474
N23	-1.898339	2.657141	-0.166724
H24	-0.895369	2.569313	-0.053129

H25	-2.290575	3.578361	-0.250626
C26	-4.108982	1.725778	-0.270788
H27	-4.577538	2.692074	-0.385638
C28	-5.067466	-1.855611	-0.044252
H29	-4.748691	-2.532227	-0.836233
H30	-4.926733	-2.350916	0.916122
H31	-6.117225	-1.599741	-0.177835
C32	5.524112	-1.179490	-0.686201
H33	6.047187	-1.603682	0.170820
H34	5.040082	-1.976730	-1.249034
H35	6.228863	-0.656346	-1.330454
H36	2.426659	2.430251	0.188048

WC-[9MG + H_{O6}]$^+$·1MC

C1	-1.434885	1.041919	-0.173307
C2	-2.791822	0.867764	-0.123451
H3	0.393558	0.089666	-0.070360
C4	-1.190491	-1.320235	0.077257
C5	-4.885904	0.997544	-0.079826
N6	-0.650116	-0.049742	-0.069130
N7	-3.840927	1.758526	-0.196140
N8	-4.596661	-0.350086	0.066191
N9	-2.499553	-1.542371	0.139908
C10	-3.243132	-0.451583	0.040166
N11	-0.335975	-2.328632	0.161594
H12	-0.729753	-3.250839	0.247345
H13	0.676634	-2.203419	0.017614
O14	-0.819371	2.205876	-0.312914
H15	-5.910289	1.343342	-0.091414
C16	2.888329	-0.772245	-0.104138
N17	2.203283	0.398636	0.009144
C18	2.860248	1.544449	0.173475
C19	4.943295	0.421861	0.116457
N20	4.283065	-0.747207	-0.055935
H21	6.023910	0.360686	0.149536
O22	2.328638	-1.856833	-0.247175
N23	2.144569	2.672524	0.282004
H24	1.143572	2.643584	0.166543
H25	2.599122	3.563245	0.377048
C26	4.283519	1.595389	0.239658
H27	4.815476	2.525338	0.376271
C28	4.988825	-2.021724	-0.188807
H29	4.672090	-2.704148	0.599010
H30	4.761821	-2.473049	-1.154113
H31	6.058865	-1.837551	-0.109359
C32	-5.538030	-1.448986	0.225271
H33	-5.364419	-2.197343	-0.547644
H34	-5.416385	-1.906252	1.207291
H35	-6.548901	-1.056308	0.128739
H36	-1.482952	2.904246	-0.395785

[9MG + H_{O6}]$^+$

C1	1.117259	1.241177	0.001616
C2	-0.226031	0.968591	-0.000662
C3	1.501863	-1.140001	-0.001207
C4	-2.323502	0.950895	-0.004310
N5	1.955205	0.166876	0.001566
N6	-1.331507	1.787027	-0.001574
N7	-1.943205	-0.384111	-0.007569
N8	0.223137	-1.443377	-0.002800
C9	-0.592091	-0.389639	-0.002986
N10	2.422973	-2.110894	-0.001616
H11	2.096758	-3.063848	-0.002524
H12	3.413784	-1.941573	-0.000851
O13	1.709931	2.405834	0.004459
H14	-3.369292	1.225605	-0.006686
C15	-2.813567	-1.554139	0.010414
H16	-2.489357	-2.258359	-0.754533
H17	-2.777005	-2.032935	0.988954
H18	-3.831752	-1.232966	-0.201664
H19	1.059326	3.121342	0.004123
H20	2.948284	0.366116	0.004264

WC-TS-PT1

C1	1.315944	0.956057	0.380166
C2	2.681106	0.805070	0.316435
H3	-0.771700	0.139139	0.051640
C4	1.073863	-1.276086	-0.273570
C5	4.775758	0.948215	0.283740
N6	0.512672	-0.067619	0.079511
N7	3.727721	1.671292	0.545889
N8	4.488871	-0.346056	-0.111858
N9	2.379523	-1.503509	-0.385298
C10	3.132731	-0.453226	-0.092283
N11	0.222542	-2.277958	-0.547363
H12	0.648153	-3.175326	-0.712751
H13	-0.712257	-2.257764	-0.145514
O14	0.716067	2.105550	0.707191
H15	5.799075	1.289989	0.353989
C16	-2.809441	-0.762555	0.288821
N17	-2.049325	0.341359	-0.020060
C18	-2.603717	1.486796	-0.440902
C19	-4.755154	0.502687	-0.271975
N20	-4.193319	-0.642874	0.175552
H21	-5.835327	0.506367	-0.349006
O22	-2.313473	-1.815662	0.643818
N23	-1.810213	2.523715	-0.711288
H24	-0.844813	2.520473	-0.408407
H25	-2.215885	3.400312	-0.991406
C26	-4.012363	1.585619	-0.600943
H27	-4.476661	2.496307	-0.948569
C28	-4.993336	-1.819038	0.527726
H29	-4.718132	-2.657134	-0.111526
H30	-4.807074	-2.091273	1.565792
H31	-6.045650	-1.577846	0.390251
C32	5.430308	-1.401719	-0.450972
H33	5.455907	-2.154135	0.337821
H34	5.128795	-1.870031	-1.387360
H35	6.419717	-0.962632	-0.569329
H36	1.391598	2.755080	0.943264

WC-[9MG + H_{O6} – H_{N1}]·[1MC + $H_{N3'}$]$^+$

C1	-1.407646	0.960030	-0.224292
C2	-2.780536	0.832519	-0.165808
H3	1.164011	0.176064	-0.085070
C4	-1.192844	-1.304905	0.131399
C5	-4.875474	0.993758	-0.129874
N6	-0.607979	-0.082250	-0.074699
N7	-3.816234	1.734385	-0.281546
N8	-4.605521	-0.344502	0.080797
N9	-2.502238	-1.548351	0.209026
C10	-3.246898	-0.462193	0.059365
N11	-0.358466	-2.352603	0.293843
H12	-0.784688	-3.262507	0.338550
H13	0.609376	-2.285784	0.008558
O14	-0.815512	2.156856	-0.426197
H15	-5.894354	1.354108	-0.159228
C16	2.968182	-0.825893	-0.190426
N17	2.211042	0.324558	-0.029982
C18	2.721478	1.545005	0.235641
C19	4.879887	0.551600	0.205377
N20	4.343366	-0.659641	-0.070055
H21	5.959208	0.582627	0.288448
O22	2.470155	-1.901208	-0.417104
N23	1.897797	2.570062	0.362707
H24	0.899891	2.481739	0.168739
H25	2.271174	3.485022	0.553871
C26	4.128217	1.667683	0.367992
H27	4.586218	2.621857	0.579667
C28	5.167115	-1.862743	-0.236741
H29	4.895157	-2.600458	0.517082
H30	4.999765	-2.287412	-1.225648
H31	6.213039	-1.585171	-0.123621
C32	-5.558219	-1.422889	0.282028
H33	-5.433543	-2.179773	-0.492715
H34	-5.405033	-1.880201	1.259803
H35	-6.565508	-1.012447	0.227614
H36	-1.503800	2.823711	-0.548257

[9MG + H_{O6} – H_{N1}]

C1	1.187928	1.187870	0.002429
C2	-0.189969	0.944088	0.005472
C3	1.543546	-1.071948	0.004265
C4	-2.299045	0.939393	-0.004868
N5	2.038545	0.185872	0.001727
N6	-1.296411	1.769824	0.002619
N7	-1.926425	-0.388209	-0.011380
N8	0.260452	-1.444703	-0.004575
C9	-0.557492	-0.395768	-0.002048
N10	2.476450	-2.064591	0.046561
H11	2.170271	-2.999051	-0.159270
H12	3.427746	-1.810160	-0.153019
O13	1.690321	2.423798	-0.002739
H14	-3.342982	1.220775	-0.009118
C15	-2.783612	-1.554685	0.007378
H16	-2.480360	-2.247027	-0.778586
H17	-2.717030	-2.063114	0.971012
H18	-3.812713	-1.240348	-0.165964
H19	0.956088	3.047486	-0.003582

Cartesian coordinates for the structures in Figure 8, optimized at ωB97XD/6-311++ G(d,p).

WC-[9MG + H_{N7}]$^+$·1MC·H_2O

C1	-1.264446	0.787026	-0.051738
C2	-2.638948	0.400939	-0.024158
H3	0.589331	-0.115616	-0.053136
C4	-0.864128	-1.633641	-0.013735
C5	-4.818807	0.264528	0.026696
N6	-0.438224	-0.320673	-0.045572
N7	-3.816305	1.119913	-0.015200
N8	-4.350172	-0.994431	0.044707
N9	-2.149912	-1.980663	0.021099
C10	-2.967005	-0.937176	0.014708
N11	0.071012	-2.570807	-0.016936
H12	-0.240687	-3.527205	0.004216
H13	1.079050	-2.352801	-0.060088
O14	-0.817375	1.934623	-0.075846
H15	-5.863974	0.527889	0.043545
C16	3.177531	-0.784228	-0.049199
N17	2.370112	0.306482	-0.022705
C18	2.886278	1.531388	0.053689
C19	5.084234	0.646250	0.085575
N20	4.561176	-0.601162	0.005186
H21	6.164496	0.710195	0.126309
O22	2.742831	-1.933260	-0.117779
N23	2.041090	2.566932	0.073353
H24	1.037728	2.407292	0.020024
H25	2.390238	3.506820	0.131020
C26	4.297419	1.744904	0.113647
H27	4.724375	2.734925	0.178946
C28	5.405600	-1.793766	-0.031789
H29	5.141970	-2.459064	0.789502
H30	5.257363	-2.324765	-0.971881
H31	6.446797	-1.488448	0.059920
C32	-5.129337	-2.226138	0.107756
H33	-4.798560	-2.894719	-0.685442
H34	-4.974327	-2.706306	1.073390
H35	-6.182938	-1.986978	-0.024951
H36	-3.843692	2.157255	-0.043767
O37	-3.021153	3.652617	-0.029886
H38	-2.090994	3.375866	-0.078346
H39	-3.102384	4.524165	-0.417397

H_2O

O1	0.000000	0.000000	0.116335
H2	0.000000	0.760673	-0.465340
H3	0.000000	-0.760673	-0.465340

WC-TS_PT1·H_2O

C1	-1.158895	0.732699	-0.165044
C2	-2.540863	0.380178	-0.104180
H3	1.007992	-0.031365	-0.046073
C4	-0.777620	-1.610939	0.116643
C5	-4.723455	0.275979	-0.012030
N6	-0.311392	-0.331748	-0.049813
N7	-3.712089	1.109177	-0.165097
N8	-4.267616	-0.976913	0.152250
N9	-2.063781	-1.967764	0.213869
C10	-2.883345	-0.936702	0.098822
N11	0.134845	-2.585120	0.210977
H12	-0.219399	-3.525552	0.256014
H13	1.092323	-2.428841	-0.099103
O14	-0.739267	1.902520	-0.294431
H15	-5.765616	0.551021	-0.020032
C16	3.095687	-0.767284	-0.277525
N17	2.230015	0.259387	0.009240
C18	2.664088	1.467661	0.414699
C19	4.904494	0.682661	0.300432
N20	4.459281	-0.518743	-0.139249
H21	5.977833	0.787034	0.397749
O22	2.713844	-1.866675	-0.637727
N23	1.774110	2.421651	0.638593
H24	0.794309	2.297569	0.339720
H25	2.092601	3.332283	0.922737
C26	4.059556	1.694980	0.594805
H27	4.430753	2.650737	0.933450
C28	5.372567	-1.619309	-0.453223
H29	5.188541	-2.457839	0.217914
H30	5.213052	-1.948405	-1.479094
H31	6.395012	-1.266047	-0.332420
C32	-5.056582	-2.184777	0.359221
H33	-4.765092	-2.929006	-0.380410
H34	-4.868793	-2.576972	1.358198
H35	-6.112237	-1.944169	0.246049
H36	-3.730754	2.134328	-0.325326
O37	-2.883088	3.614988	-0.522819
H38	-1.975533	3.256779	-0.524132
H39	-2.924314	4.331406	-1.156531

WC-[9MG + H_{N7} – H_{N1}]·[1MC + $H_{N3'}$]$^+$·H_2O

C1	-1.203083	0.695794	-0.089173
C2	-2.598404	0.392155	-0.042763
H3	1.318226	-0.011194	-0.067507
C4	-0.895170	-1.643872	0.012265
C5	-4.786162	0.344059	0.032371
N6	-0.386970	-0.381724	-0.059719
N7	-3.749203	1.156592	-0.044277
N8	-4.368043	-0.931114	0.085456
N9	-2.192437	-1.986922	0.071159
C10	-2.981634	-0.928061	0.041019
N11	-0.009340	-2.652026	0.037257
H12	-0.368607	-3.590321	0.044983
H13	0.980782	-2.489530	-0.095909
O14	-0.756113	1.874038	-0.147200
H15	-5.819395	0.650226	0.048852
C16	3.217228	-0.841249	-0.121138
N17	2.355673	0.234013	-0.025317
C18	2.744615	1.517237	0.157519
C19	4.992676	0.732790	0.167255

N20	4.570839	-0.542377	-0.024164
H21	6.064567	0.868768	0.238232
O22	2.826779	-1.975713	-0.278167
N23	1.826030	2.453088	0.227040
H24	0.807646	2.234881	0.093224
H25	2.114788	3.407166	0.367477
C26	4.140598	1.778087	0.264671
H27	4.506533	2.782645	0.413784
C28	5.505003	-1.666983	-0.130388
H29	5.303664	-2.390372	0.658812
H30	5.384988	-2.155031	-1.096886
H31	6.518876	-1.284207	-0.031805
C32	-5.192327	-2.127451	0.189562
H33	-4.899977	-2.827606	-0.591632
H34	-5.040720	-2.592650	1.163236
H35	-6.238545	-1.852034	0.067372
H36	-3.739056	2.190737	-0.112426
O37	-2.832128	3.659142	-0.180906
H38	-1.949099	3.240116	-0.218140
H39	-2.838849	4.396917	-0.790723

WC-TS_enol·H_2O

C1	-1.294699	0.776359	-0.087632
C2	-2.660256	0.436784	-0.036441
H3	0.565650	-0.106194	-0.086621
C4	-0.902861	-1.619836	-0.018733
C5	-4.796039	0.369153	0.053238
N6	-0.463218	-0.307002	-0.075683
N7	-3.803362	1.217886	-0.020754
N8	-4.373579	-0.926642	0.084528
N9	-2.187421	-1.951463	0.040009
C10	-3.002717	-0.903335	0.030747
N11	0.028625	-2.563302	-0.021714
H12	-0.289977	-3.516884	0.014577
H13	1.034737	-2.354123	-0.099149
O14	-0.816481	1.946479	-0.138274
H15	-5.842180	0.633745	0.086822
C16	3.150565	-0.798537	-0.084966
N17	2.355786	0.301983	-0.026356
C18	2.888414	1.513853	0.110240
C19	5.073335	0.599498	0.139169
N20	4.535654	-0.635434	-0.002627
H21	6.153516	0.647182	0.199560
O22	2.702889	-1.937072	-0.205742
N23	2.056716	2.560990	0.160847
H24	1.055807	2.416865	0.072523
H25	2.416455	3.492890	0.264165
C26	4.299958	1.706576	0.201851
H27	4.737905	2.687366	0.315177
C28	5.364674	-1.837613	-0.072258
H29	5.085506	-2.525894	0.724652
H30	5.216581	-2.335597	-1.030164
H31	6.409034	-1.549639	0.037308
C32	-5.193478	-2.126300	0.182360
H33	-4.892916	-2.830603	-0.592205
H34	-5.061751	-2.588554	1.160672
H35	-6.237968	-1.852990	0.041907
H36	-3.444835	2.621452	-0.079112
O37	-2.741707	3.447919	-0.094922
H38	-1.804346	2.901258	-0.135469
H39	-2.864614	4.022389	-0.856351

WC-[9MG + H_{O6}]$^+$·1MC·H_2O

C1	-1.333567	0.735556	-0.118269
C2	-2.685986	0.439254	-0.056307
H3	0.547277	-0.100133	-0.078716
C4	-0.910574	-1.629072	0.023716
C5	-4.801031	0.355146	0.032734
N6	-0.480936	-0.316257	-0.072244
N7	-3.832544	1.217105	-0.066640
N8	-4.377443	-0.951069	0.106876
N9	-2.195378	-1.955458	0.093431
C10	-3.017091	-0.917829	0.053833
N11	0.021740	-2.569573	0.050742
H12	-0.297360	-3.522450	0.103782
H13	1.022629	-2.360973	-0.083506
O14	-0.783822	1.912894	-0.212864
H15	-5.852631	0.603258	0.056901
C16	3.122798	-0.794966	-0.125085
N17	2.346897	0.313706	0.011835
C18	2.908034	1.503530	0.215877
C19	5.074847	0.550607	0.153963
N20	4.511015	-0.662133	-0.057009
H21	6.156513	0.574808	0.199085
O22	2.653180	-1.916635	-0.305418
N23	2.101901	2.564801	0.346616
H24	1.104879	2.454224	0.228288
H25	2.481589	3.484457	0.483823
C26	4.322996	1.664638	0.299378
H27	4.779769	2.629049	0.465833
C28	5.315900	-1.873612	-0.209576
H29	5.045332	-2.596406	0.559269
H30	5.134359	-2.319910	-1.186826
H31	6.367642	-1.609001	-0.113503
C32	-5.194858	-2.148527	0.235380
H33	-4.898934	-2.872017	-0.523406
H34	-5.063959	-2.588292	1.224303
H35	-6.239360	-1.877459	0.090552
H36	-3.402799	3.060246	-0.201551
O37	-2.631170	3.660130	-0.232126
H38	-1.474275	2.659265	-0.255458
H39	-2.791728	4.334011	-0.894718

WC-TS-enol_PT1·H_2O

C1	1.212237	0.681868	0.241977
C2	2.573772	0.410763	0.154227
H3	-0.939150	-0.023810	0.038080
C4	0.797126	-1.600140	-0.157889
C5	4.690161	0.344886	0.035438
N6	0.342117	-0.324867	0.074781
N7	3.718906	1.184989	0.250621
N8	4.269088	-0.940642	-0.198874

N9	2.076801	-1.936317	-0.282760
C10	2.906785	-0.915761	-0.127636
N11	-0.132218	-2.560273	-0.293783
H12	0.221492	-3.499416	-0.372656
H13	-1.052766	-2.425124	0.118069
O14	0.676733	1.867957	0.451637
H15	5.740785	0.598088	0.035707
C16	-3.029790	-0.745844	0.357177
N17	-2.185925	0.256908	-0.058222
C18	-2.646532	1.390482	-0.608653
C19	-4.868669	0.591193	-0.373974
N20	-4.399490	-0.537397	0.205810
H21	-5.944537	0.666907	-0.470663
O22	-2.619494	-1.787046	0.835787
N23	-1.773397	2.327942	-0.970242
H24	-0.814987	2.283219	-0.638198
H25	-2.108124	3.197718	-1.348182
C26	-4.043209	1.573346	-0.804012
H27	-4.434480	2.472970	-1.255024
C28	-5.289699	-1.604696	0.668567
H29	-5.083185	-2.523251	0.120238
H30	-5.125005	-1.784828	1.730052
H31	-6.319702	-1.296023	0.500198
C32	5.085194	-2.109336	-0.487944
H33	4.800226	-2.923830	0.177238
H34	4.941570	-2.421155	-1.522767
H35	6.131669	-1.856720	-0.324168
H36	3.301887	2.979453	0.609628
O37	2.549841	3.597107	0.717731
H38	1.370998	2.585840	0.606655
H39	2.721218	4.152861	1.479571

WC-[9MG + H_{O6} – H_{N1}]·[1MC + $H_{N3'}$]$^{+}$·H_2O

C1	1.283022	0.654108	0.202316
C2	2.653085	0.412076	0.096460
H3	-1.305176	0.030619	0.115161
C4	0.903479	-1.621489	-0.051327
C5	4.770669	0.371363	-0.050410
N6	0.422740	-0.354832	0.121182
N7	3.787074	1.208944	0.120220
N8	4.368544	-0.932357	-0.186160
N9	2.186437	-1.962701	-0.171009
C10	3.004283	-0.923738	-0.096345
N11	-0.011660	-2.609785	-0.132421
H12	0.343935	-3.550374	-0.150616
H13	-0.957974	-2.456538	0.190567
O14	0.745821	1.861111	0.368755
H15	5.816368	0.641620	-0.086365
C16	-3.187275	-0.814705	0.267921
N17	-2.339224	0.252564	0.022584
C18	-2.743158	1.473254	-0.388525
C19	-4.973509	0.653302	-0.336040
N20	-4.541986	-0.558295	0.087624
H21	-6.044179	0.755897	-0.461486
O22	-2.780876	-1.897756	0.613979
N23	-1.836506	2.410984	-0.586877
H24	-0.855782	2.264748	-0.327085
H25	-2.127052	3.325787	-0.889756
C26	-4.132637	1.684936	-0.587927
H27	-4.508180	2.641699	-0.917635
C28	-5.462701	-1.672426	0.339405
H29	-5.275104	-2.475002	-0.373421
H30	-5.309821	-2.051022	1.348794
H31	-6.482544	-1.309309	0.229695
C32	5.199899	-2.105259	-0.397024
H33	4.963141	-2.859950	0.352569
H34	5.023698	-2.518827	-1.390421
H35	6.245788	-1.816643	-0.302415
H36	3.358717	2.990486	0.369406
O37	2.623014	3.630637	0.479165
H38	1.438091	2.585028	0.459901
H39	2.833523	4.199658	1.220889

WC-TS1

C1	-1.828351	1.173701	0.067575
C2	-3.194600	0.743576	0.017067
H3	0.054040	0.309356	0.094320
C4	-1.370607	-1.239912	0.037792
C5	-5.380233	0.550630	-0.075244
N6	-0.976127	0.080139	0.077246
N7	-4.389809	1.430010	-0.017579
N8	-4.876263	-0.689262	-0.081221
N9	-2.651547	-1.621891	-0.013871
C10	-3.491290	-0.598893	-0.023256
N11	-0.415263	-2.153290	0.052008
H12	-0.705477	-3.115894	0.015599
H13	0.593527	-1.904977	0.103220
O14	-1.439017	2.329926	0.096397
H15	-6.430134	0.791064	-0.112876
C16	2.639325	-0.313132	0.054124
N17	1.784827	0.748480	0.059439
C18	2.275474	1.987860	-0.007927
C19	4.475101	1.124242	-0.109108
N20	3.996753	-0.135186	-0.084646
H21	5.555094	1.226187	-0.180961
O22	2.203613	-1.477610	0.184009
N23	1.407965	3.009312	-0.003593
H24	0.407160	2.838349	0.049595
H25	1.741254	3.955308	-0.049192
C26	3.678025	2.226181	-0.074571
H27	4.085458	3.226508	-0.117568
C28	4.964106	-1.908546	1.121337
H29	5.215117	-1.032180	1.700991
H30	3.918999	-2.195279	1.031597
H31	5.721484	-2.668540	1.014579
C32	-5.619807	-1.944053	-0.125294
H33	-5.245417	-2.546446	-0.951507
H34	-5.472815	-2.482085	0.810397
H35	-6.676501	-1.727226	-0.270964
O36	5.532454	-2.047276	-1.021570
H37	6.394620	-1.743899	-1.319884
H38	4.911024	-1.293602	-1.094040

H39 -4.490442 2.434924 -0.003442

WC-[9MG + H_{N7}]$^+$·1HC

C1 0.979698 1.095237 0.001276
C2 2.402029 0.932372 0.001868
H3 -0.695281 -0.104528 -0.000765
C4 0.990117 -1.363387 -0.002051
C5 4.585933 1.157474 0.007119
N6 0.352160 -0.141639 -0.000655
N7 3.445608 1.833415 0.006344
N8 4.327844 -0.155547 0.003892
N9 2.318966 -1.494238 -0.003111
C10 2.949902 -0.329573 -0.000306
N11 0.224441 -2.442982 -0.002678
H12 0.687727 -3.336190 -0.003558
H13 -0.805808 -2.392049 0.000454
O14 0.372251 2.154090 0.002286
H15 5.571037 1.594882 0.010663
C16 -3.128209 -1.140997 0.003835
N17 -2.501384 0.062640 -0.000659
C18 -3.207701 1.193645 -0.004379
C19 -5.254503 -0.009065 0.000730
N20 -4.518685 -1.148463 0.004880
H21 -6.330474 -0.127164 0.001718
O22 -2.532059 -2.214810 0.007002
N23 -2.538600 2.347013 -0.008362
H24 -1.519673 2.348974 -0.005873
H25 -3.031004 3.222755 -0.010525
C26 -4.643399 1.193272 -0.004240
H27 -5.209878 2.112880 -0.007577
C28 5.299427 -1.245479 -0.010363
H29 5.071921 -1.929717 0.805415
H30 5.230520 -1.776639 -0.958902
H31 6.297993 -0.831396 0.116454
H32 3.355085 2.839475 0.011098
H33 -4.955913 -2.057910 0.008603

CH_3OH

C1 0.661363 -0.020245 0.000001
H2 1.082520 0.985326 0.000098
H3 1.024454 -0.544778 0.892371
H4 1.024458 -0.544594 -0.892477
O5 -0.744663 0.121755 0.000002
H6 -1.142307 -0.748524 -0.000012

WC-TS1_PT1

C1 0.888551 1.027155 -0.144807
C2 2.311904 0.899405 -0.117998
H3 -1.129929 -0.076934 -0.049589
C4 0.912069 -1.354731 0.090065
C5 4.492030 1.165672 -0.083766
N6 0.230243 -0.170707 -0.039593
N7 3.340609 1.815409 -0.185885
N8 4.255042 -0.144817 0.052901
N9 2.247272 -1.494860 0.144251
C10 2.879027 -0.340889 0.035979
N11 0.190252 -2.472279 0.185612
H12 0.696627 -3.339971 0.227992
H13 -0.810693 -2.476281 -0.002995
O14 0.316353 2.119952 -0.245453
H15 5.469789 1.618087 -0.109106
C16 -3.073650 -1.150318 -0.182926
N17 -2.383693 0.028689 -0.036918
C18 -3.023896 1.203251 0.153115
C19 -5.126828 0.085270 0.097821
N20 -4.456731 -1.073692 -0.117784
H21 -6.206309 0.019048 0.141069
O22 -2.535684 -2.226468 -0.359231
N23 -2.313267 2.308661 0.254630
H24 -1.289031 2.300322 0.084295
H25 -2.786915 3.187198 0.381051
C26 -4.454310 1.243154 0.242999
H27 -4.969330 2.177784 0.407160
C28 5.241854 -1.208262 0.203661
H29 5.112530 -1.683268 1.175382
H30 5.090523 -1.947335 -0.581858
H31 6.239728 -0.780326 0.125942
H32 3.231395 2.812732 -0.299740
H33 -4.942347 -1.951987 -0.227499

WC-[9MG + H_{N7} – H_{N1}]·[1HC + $H_{N3'}$]$^+$

C1 0.919133 0.988136 0.008116
C2 2.347259 0.901410 0.006817
H3 -1.430518 -0.083913 0.005686
C4 0.996703 -1.377480 -0.002594
C5 4.524628 1.208700 0.007749
N6 0.290256 -0.214396 0.003613
N7 3.358059 1.840200 0.012059
N8 4.315868 -0.113503 0.000310
N9 2.337532 -1.510087 -0.007137
C10 2.943237 -0.337515 -0.001391
N11 0.288543 -2.515579 -0.005572
H12 0.790314 -3.385922 -0.007074
H13 -0.723664 -2.509709 0.004425
O14 0.318773 2.082333 0.012713
H15 5.492785 1.681684 0.010841
C16 -3.186257 -1.187541 0.010410
N17 -2.496360 0.008711 0.003856
C18 -3.081615 1.231960 -0.008557
C19 -5.202172 0.140940 -0.008983
N20 -4.565137 -1.059113 0.004429
H21 -6.284112 0.106912 -0.013550
O22 -2.642737 -2.266086 0.020491
N23 -2.317754 2.295640 -0.013112
H24 -1.262640 2.223426 -0.003405
H25 -2.750961 3.204797 -0.022471
C26 -4.511999 1.299292 -0.015962
H27 -5.015662 2.253962 -0.026511
C28 5.325176 -1.165030 -0.021646
H29 5.124226 -1.863188 0.789553
H30 5.274914 -1.694642 -0.972467
H31 6.309301 -0.717498 0.106166

H32	3.227149	2.841007	0.021038
H33	-5.081031	-1.927247	0.009259

WC-TS2

C1	-0.867780	1.422840	-0.043019
C2	-2.289747	1.293959	-0.052258
H3	0.778075	0.179794	-0.043790
C4	-0.932502	-1.033313	-0.094773
C5	-4.463777	1.532873	-0.080517
N6	-0.266657	0.171332	-0.058777
N7	-3.313190	2.217328	-0.057821
N8	-4.256088	0.219573	-0.079946
N9	-2.257196	-1.133129	-0.108485
C10	-2.885862	0.053213	-0.074248
N11	-0.180139	-2.130102	-0.120387
H12	-0.654840	-3.015872	-0.109915
H13	0.848929	-2.095919	-0.099011
O14	-0.226807	2.464702	-0.022110
H15	-5.431155	2.011258	-0.088327
C16	3.215254	-0.916619	-0.006037
N17	2.606494	0.295047	0.002123
C18	3.321078	1.417582	0.054180
C19	5.338773	0.172812	0.098819
N20	4.611224	-0.970251	0.046485
H21	6.414295	0.051905	0.136939
O22	2.591518	-1.976372	-0.056840
N23	2.665025	2.580308	0.058552
H24	1.645481	2.596699	0.026222
H25	3.169208	3.448003	0.099321
C26	4.750278	1.388662	0.104863
H27	5.338072	2.293961	0.147569
C28	5.242051	-2.287658	0.034354
H29	4.873840	-2.882424	0.869572
H30	5.004749	-2.807023	-0.894065
H31	6.320024	-2.159232	0.120326
C32	-5.155645	-1.759697	-1.004657
H33	-5.958216	-2.445359	-0.786387
H34	-5.337983	-0.975094	-1.723456
H35	-4.129731	-2.067605	-0.811919
O36	-5.704911	-1.662961	1.192648
H37	-5.260594	-0.817067	1.329751
H38	-6.590759	-1.597999	1.561468
H39	-3.206850	3.220344	-0.036343

WC-[9HG + H_{N7}]$^{+}$·1MC

C1	1.718800	0.935657	-0.000131
C2	3.104144	0.568220	-0.000061
H3	-0.114419	-0.010320	-0.000075
C4	1.374647	-1.498277	0.000090
C5	5.302300	0.493142	-0.000009
N6	0.918854	-0.197082	-0.000056
N7	4.265904	1.313594	-0.000115
N8	4.850655	-0.769059	0.000115
N9	2.672320	-1.820016	0.000169
C10	3.462835	-0.761755	0.000085
N11	0.464575	-2.456514	0.000157
H12	0.797793	-3.406174	0.000240
H13	-0.549546	-2.256925	0.000002
O14	1.274501	2.071708	-0.000244
H15	6.339003	0.786939	-0.000022
C16	-2.666409	-0.700661	-0.000081
N17	-1.878241	0.403609	-0.000011
C18	-2.414866	1.623222	0.000093
C19	-4.598436	0.700592	0.000166
N20	-4.053096	-0.540496	0.000063
H21	-5.680357	0.747068	0.000230
O22	-2.210014	-1.844253	-0.000263
N23	-1.589353	2.673224	0.000109
H24	-0.581073	2.534821	-0.000025
H25	-1.956100	3.608354	0.000145
C26	-3.831127	1.812964	0.000193
H27	-4.275924	2.797260	0.000285
C28	-4.876912	-1.748012	-0.000182
H29	-4.660556	-2.344300	-0.886113
H30	-4.659215	-2.345520	0.884585
H31	-5.925937	-1.455975	0.000816
H32	4.313134	2.323421	-0.000223
H33	5.426110	-1.599663	0.000212

WC-TS2_PT1

C1	1.615965	0.868034	0.169120
C2	3.006430	0.531596	0.125841
H3	-0.526328	0.066723	0.028437
C4	1.289680	-1.479184	-0.180605
C5	5.206021	0.494350	0.085000
N6	0.790218	-0.215525	0.011804
N7	4.157362	1.286736	0.229091
N8	4.772889	-0.759214	-0.115046
N9	2.590454	-1.810479	-0.255693
C10	3.383758	-0.771165	-0.096509
N11	0.411428	-2.471450	-0.321525
H12	0.786993	-3.400637	-0.406563
H13	-0.574557	-2.338313	-0.097576
O14	1.211349	2.025258	0.323345
H15	6.238051	0.800778	0.124615
C16	-2.614292	-0.714101	0.159179
N17	-1.764640	0.355060	0.016905
C18	-2.226861	1.606767	-0.178058
C19	-4.456125	0.778325	-0.134492
N20	-3.983258	-0.471762	0.088198
H21	-5.532894	0.879275	-0.187086
O22	-2.215397	-1.852102	0.340062
N23	-1.363391	2.602817	-0.275526
H24	-0.360600	2.455026	-0.071170
H25	-1.709187	3.539445	-0.396823
C26	-3.631175	1.837178	-0.277804
H27	-4.021964	2.829778	-0.445054
C28	-4.874351	-1.622617	0.245795
H29	-4.670487	-2.358987	-0.530806
H30	-4.713441	-2.085061	1.218908
H31	-5.903390	-1.276845	0.166139
H32	4.187491	2.283397	0.393344

H33 5.360964 -1.568207 -0.255868

WC-[9HG + H_{N7} – H_{N1}]·[1MC + $H_{N3'}$]$^+$

C1 1.652988 0.835710 0.008799
C2 3.056827 0.551819 0.003711
H3 -0.840839 0.101266 0.007144
C4 1.406403 -1.517206 -0.002273
C5 5.259279 0.577770 -0.003958
N6 0.865805 -0.269073 0.005766
N7 4.184307 1.348354 0.004027
N8 4.866791 -0.704787 -0.009726
N9 2.717517 -1.834539 -0.008505
C10 3.477532 -0.759070 -0.005119
N11 0.549674 -2.546825 -0.005009
H12 0.927857 -3.477686 -0.008079
H13 -0.452219 -2.399574 0.005308
O14 1.212510 2.001944 0.015045
H15 6.280516 0.920145 -0.005509
C16 -2.722874 -0.752706 0.005815
N17 -1.879044 0.340156 0.002875
C18 -2.288018 1.631180 -0.003176
C19 -4.526092 0.815623 -0.013226
N20 -4.082273 -0.467149 -0.007052
H21 -5.601584 0.941435 -0.019889
O22 -2.311911 -1.891246 0.017952
N23 -1.385002 2.583002 -0.001116
H24 -0.354252 2.369072 0.006143
H25 -1.690468 3.542295 -0.005418
C26 -3.691395 1.878816 -0.011876
H27 -4.075180 2.887791 -0.018060
C28 -4.999213 -1.610641 0.003877
H29 -4.773606 -2.269267 -0.833452
H30 -4.886560 -2.167354 0.933848
H31 -6.017734 -1.237521 -0.083736
H32 4.181656 2.358457 0.009753
H33 5.480580 -1.506380 -0.016305