Supporting Information

Experimental and Theoretical Assessment of Protonated Hoogsteen 9-Methylguanine–1-Methylcytosine Base-Pair Dissociation: Kinetics within a Statistical Reaction Framework

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

HG-[9MG·1MC + H]$^+$_1
(HG-9MG·[1MC + $H_{N3'}$]$^+$)

C1	-1.931107	-1.442366	-0.010694
C2	-1.638144	-0.055147	-0.010444
C3	-4.278253	-0.677256	-0.000014
C4	-0.737374	1.872188	-0.005478
N5	-0.430335	0.601092	-0.013268
N6	-2.088534	2.087400	0.001194
N7	-4.000617	0.601410	-0.000999
C8	-2.678672	0.854920	-0.000007
N9	-5.566188	-1.083732	0.037968
H10	-6.268035	-0.367623	-0.048263
H11	-5.832574	-2.028028	-0.179049
O12	-1.156018	-2.394576	-0.011510
H13	-0.016478	2.677130	-0.006253
C14	-2.781902	3.366019	0.029407
H15	-3.526692	3.394337	-0.765050
H16	-3.275083	3.504250	0.991815
H17	-2.053678	4.160535	-0.125440
H18	1.132254	-0.015499	-0.013828
C19	2.531665	-1.592540	0.006385
C20	3.926580	-1.873955	0.019813
C21	4.785584	-0.827032	0.019140
H22	4.289514	-2.890509	0.031626
H23	5.857734	-0.979767	0.029503
N24	2.156645	-0.298596	-0.006743
C25	3.018959	0.786851	-0.010814
O26	2.621424	1.924408	-0.027356
N27	4.375324	0.464410	0.006714
C28	5.318964	1.585254	-0.006260
H29	5.224882	2.137999	-0.940781
H30	5.102168	2.255270	0.824420
H31	6.328306	1.190160	0.091029
N32	1.609767	-2.535171	0.006756
H33	1.901005	-3.498815	0.016592
H34	0.591852	-2.353101	-0.002346
N35	-3.314579	-1.661376	-0.004394
H36	-3.586596	-2.634662	0.030152

HG-[9MG·1MC + H]$^+$_2
(HG-[9MG + H_{N7}]$^+$·1MC)

C1	-1.927032	-1.493369	-0.004072
C2	-1.602540	-0.105503	-0.003303
C3	-4.251501	-0.635894	0.002855
C4	-0.638193	1.839850	-0.007520
N5	-0.394384	0.547671	-0.007942
N6	-1.969314	2.065507	-0.003858
N7	-3.925935	0.636725	0.003658
C8	-2.601079	0.840975	0.000032
N9	-5.548506	-0.985119	0.005539
H10	-6.232983	-0.247761	0.009047
H11	-5.863027	-1.938848	0.005423
O12	-1.180810	-2.453724	-0.007158
H13	0.137063	2.591660	-0.010631
C14	-2.638699	3.361323	0.013394
H15	-3.369380	3.398139	-0.793063
H16	-3.143039	3.501624	0.968951
H17	-1.892327	4.140584	-0.128788
H18	0.601232	0.094372	-0.010218
C19	2.612949	-1.630162	0.000825
C20	4.030048	-1.806433	0.010380
C21	4.789229	-0.686567	0.011521
H22	4.483524	-2.786576	0.016984
H23	5.871413	-0.730216	0.018829
N24	2.081632	-0.409940	-0.007099
C25	2.854261	0.716103	-0.006072
O26	2.368143	1.838215	-0.013238
N27	4.243203	0.553922	0.004062
C28	5.062636	1.763996	0.002535
H29	4.859719	2.347822	-0.895019
H30	4.826265	2.371890	0.875400
H31	6.112785	1.477276	0.026484
N32	1.789058	-2.681339	-0.000166
H33	2.160389	-3.615026	0.005939
H34	0.778467	-2.563923	-0.005612
N35	-3.324031	-1.653872	-0.000416
H36	-3.631291	-2.617745	-0.000451

HG-[9MG·1MC + H]$^+$_3
(HG-9MG(*enol*)·[1MC + $H_{N3'}$]$^+$)

C1	-2.160560	-1.408917	-0.019362
C2	-1.680390	-0.102987	-0.014401
C3	-4.310891	-0.615699	0.008530
C4	-0.675117	1.776362	-0.013745
N5	-0.431273	0.489192	-0.024461
N6	-2.005836	2.072573	0.001349
N7	-3.983920	0.680183	0.015480
C8	-2.674274	0.873768	0.002836
N9	-5.619515	-0.933203	0.018896
H10	-6.306302	-0.200666	0.033872
H11	-5.901242	-1.896535	0.015997
O12	-1.306162	-2.452409	-0.035844
H13	0.091922	2.538085	-0.018222
C14	-2.624534	3.387802	0.034292
H15	-3.359053	3.464026	-0.766838
H16	-3.121205	3.543133	0.992385
H17	-1.852494	4.143148	-0.104669
H18	1.114159	-0.054591	-0.026373
C19	2.554441	-1.595821	0.010265
C20	3.947376	-1.864936	0.035764
C21	4.793577	-0.804697	0.034312
H22	4.323489	-2.876492	0.057222
H23	5.867515	-0.943790	0.053894
N24	2.156595	-0.313753	-0.014798
C25	3.004533	0.783542	-0.018135
O26	2.593483	1.915241	-0.042558
N27	4.366152	0.478360	0.010049

C28	5.294319	1.613416	-0.001520
H29	5.190665	2.164694	-0.935705
H30	5.066998	2.278829	0.829992
H31	6.309217	1.232868	0.094992
N32	1.639062	-2.554149	0.010805
H33	1.932845	-3.516334	0.029224
H34	0.637548	-2.368809	-0.008472
N35	-3.444445	-1.662743	-0.007969
H36	-1.841249	-3.256446	-0.038575

HG-[9MG·1MC + H]$^{+}$_4
(HG-[9MG + H$_{N7}$]$^{+}$(*enol*)·1MC)

C1	-2.137568	-1.450573	-0.006479
C2	-1.661858	-0.137423	-0.005795
C3	-4.284134	-0.627148	0.005787
C4	-0.644992	1.789488	-0.010574
N5	-0.431676	0.489132	-0.012399
N6	-1.962581	2.056830	-0.004167
N7	-3.944954	0.669086	0.006686
C8	-2.638175	0.848777	0.000312
N9	-5.590578	-0.932454	0.011657
H10	-6.273447	-0.195336	0.017438
H11	-5.880322	-1.894159	0.011605
O12	-1.285326	-2.479426	-0.013337
H13	0.155291	2.515258	-0.014367
C14	-2.594327	3.370845	0.014511
H15	-3.316581	3.431174	-0.798255
H16	-3.105316	3.517203	0.965640
H17	-1.826062	4.130919	-0.114887
H18	0.541482	0.044825	-0.015329
C19	2.702868	-1.636269	0.001821
C20	4.122728	-1.763674	0.015324
C21	4.838227	-0.614378	0.016023
H22	4.612342	-2.726189	0.024948
H23	5.921263	-0.614581	0.026100
N24	2.116918	-0.445601	-0.009738
C25	2.847263	0.709128	-0.008270
O26	2.322220	1.813213	-0.017366
N27	4.242599	0.601204	0.004602
C28	5.013433	1.843439	0.004513
H29	4.780547	2.423004	-0.888375
H30	4.759056	2.436590	0.882453
H31	6.074255	1.598676	0.019446
N32	1.917712	-2.723716	0.000680
H33	2.315971	-3.645857	0.009407
H34	0.912488	-2.627045	-0.008195
N35	-3.424357	-1.681101	-0.000437
H36	-1.808499	-3.291707	-0.013243

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

HG-[9MG·1MC + H]$^+$·H_2O_1

C1	-1.777697	-0.937746	-0.005328
C2	-1.278442	0.390486	-0.005302
C3	-3.978472	0.163172	0.002102
C4	-0.102620	2.165701	-0.007921
N5	0.013760	0.863260	-0.009586
N6	-1.407014	2.577187	-0.004449
N7	-3.516124	1.392247	0.003203
C8	-2.173796	1.444468	-0.001130
N9	-5.304190	-0.060244	0.005008
H10	-5.914301	0.738092	0.008417
H11	-5.678136	-0.997803	0.004416
O12	-1.143207	-1.993346	-0.007765
H13	0.727777	2.857017	-0.010767
C14	-1.907602	3.941843	0.017940
H15	-2.634177	4.077032	-0.782683
H16	-2.385912	4.149854	0.975425
H17	-1.072456	4.624967	-0.129193
H18	1.454378	0.036964	-0.010075
C19	2.604034	-1.733772	0.002541
C20	3.940983	-2.224669	0.011456
C21	4.948572	-1.320475	0.010996
H22	4.143715	-3.284846	0.018803
H23	5.985408	-1.633482	0.017726
N24	2.428935	-0.398068	-0.006172
C25	3.445798	0.542832	-0.006058
O26	3.228461	1.728426	-0.012801
N27	4.738145	0.018226	0.002461
C28	5.839205	0.983866	0.001561
H29	5.781820	1.608146	-0.889548
H30	5.772357	1.620801	0.882966
H31	6.781039	0.438605	0.010504
N32	1.550265	-2.525535	0.002556
H33	1.694560	-3.521781	0.009304
H34	0.567229	-2.193488	-0.003234
N35	-3.171487	-0.953200	-0.001526
H36	-3.617140	-1.869143	-0.001163
O37	-5.257824	-3.033611	-0.000028
H38	-5.454630	-3.578608	0.765393
H39	-5.456778	-3.575422	-0.767156

2

C1	1.957273	1.403955	-0.008390
C2	1.848791	-0.011463	-0.013404
C3	4.386524	0.949543	0.006845
C4	1.208413	-2.039473	-0.016134
N5	0.737627	-0.819974	-0.020333
N6	2.576413	-2.076461	-0.008194
N7	4.278171	-0.353404	-0.001093
C8	2.999532	-0.777170	-0.003646
N9	5.612081	1.520899	0.056943
H10	6.397497	0.898642	-0.038802
H11	5.753424	2.485381	-0.188050
O12	1.067012	2.246795	-0.008055
H13	0.599692	-2.932372	-0.019888
C14	3.430738	-3.253013	0.016668
H15	4.191090	-3.166956	-0.758767
H16	3.916050	-3.346490	0.988562
H17	2.818791	-4.133760	-0.171747
H18	-0.909887	-0.419132	-0.015553
C19	-2.511513	0.946992	-0.002523
C20	-3.935660	1.029632	0.007857
C21	-4.636435	-0.126414	0.013148
H22	-4.421341	1.993931	0.012291
H23	-5.719408	-0.129229	0.021891
N24	-1.959338	-0.284956	-0.007888
C25	-2.660805	-1.479334	-0.003568
O26	-2.107425	-2.551821	-0.009766
N27	-4.046657	-1.350703	0.008599
C28	-4.822100	-2.592313	0.011441
H29	-4.599621	-3.169627	-0.885576
H30	-4.563305	-3.187456	0.886642
H31	-5.881049	-2.342032	0.036083
N32	-1.743475	2.013670	-0.006681
H33	-2.194319	2.926715	-0.002949
H34	-0.715171	1.973325	-0.010561
N35	3.303566	1.799567	0.002907
H36	3.446880	2.799350	0.048687
O37	-3.445744	4.361043	0.002228
H38	-3.569131	4.925541	-0.763897
H39	-3.558202	4.929907	0.766801

3

C1	1.884189	-0.960662	0.030002
C2	1.411216	0.373780	0.022702
C3	4.101903	0.081886	-0.027792
C4	0.280332	2.178126	0.027850
N5	0.131304	0.879010	0.043740
N6	1.593415	2.557836	-0.001387
N7	3.671116	1.321465	-0.039271
C8	2.332019	1.407269	-0.006426
N9	5.428310	-0.164355	-0.028565
H10	6.043009	0.623805	-0.140926
H11	5.794691	-1.085160	-0.195597
O12	1.219983	-2.007087	0.052827
H13	-0.533288	2.889251	0.038658
C14	2.126530	3.910271	-0.044648
H15	2.859084	4.039531	0.751430
H16	2.605169	4.092673	-1.007057
H17	1.308192	4.614721	0.095652
H18	-1.338008	0.109235	0.048876
C19	-2.547363	-1.616274	-0.030777
C20	-3.898226	-2.060871	-0.081710
C21	-4.874811	-1.122416	-0.068392
H22	-4.136650	-3.112459	-0.131198
H23	-5.921323	-1.399000	-0.105262
N24	-2.327173	-0.289658	0.028419

C25	-3.310937	0.686108	0.038786
O26	-3.051851	1.862128	0.086111
N27	-4.619755	0.206788	-0.010345
C28	-5.688277	1.208754	0.012277
H29	-5.657352	1.760920	0.951273
H30	-5.554219	1.907419	-0.812471
H31	-6.645158	0.699904	-0.086448
N32	-1.518650	-2.442828	-0.038702
H33	-1.695365	-3.432502	-0.087844
H34	-0.529452	-2.141652	0.001669
N35	3.273831	-1.011709	0.009434
H36	3.666267	-1.959438	0.041500
O37	3.476628	-3.765015	0.001339
H38	2.515933	-3.683896	0.063809
H39	3.734163	-4.555219	0.477229

4

C1	-1.427135	-1.622635	0.005199
C2	-1.214521	-0.221196	0.013910
C3	-3.822913	-1.002964	0.020535
C4	-0.422604	1.753650	0.010608
N5	-0.045748	0.502861	0.005123
N6	-1.785186	1.891631	0.022120
N7	-3.610177	0.299345	0.032501
C8	-2.305323	0.627218	0.025989
N9	-5.074238	-1.480142	0.035915
H10	-5.835655	-0.803102	-0.019205
H11	-5.270393	-2.457818	-0.083344
O12	-0.596933	-2.527179	-0.004262
H13	0.251595	2.598123	0.004959
C14	-2.546756	3.129425	0.036513
H15	-3.273001	3.123820	-0.776432
H16	-3.064032	3.242623	0.990079
H17	-1.860350	3.963223	-0.101878
H18	1.545128	-0.026254	-0.005908
C19	3.039689	-1.514488	-0.003431
C20	4.449557	-1.708477	-0.000783
C21	5.241332	-0.609491	-0.001112
H22	4.875741	-2.700179	0.002339
H23	6.320949	-0.695614	0.000868
N24	2.585110	-0.246260	-0.006618
C25	3.377484	0.890823	-0.010167
O26	2.909455	2.001554	-0.017765
N27	4.751238	0.653930	-0.003328
C28	5.622348	1.831957	-0.015648
H29	5.482245	2.386047	-0.943533
H30	5.373665	2.479332	0.824060
H31	6.656011	1.501498	0.066246
N32	2.176606	-2.511385	-0.002466
H33	2.525470	-3.455776	-0.000489
H34	1.149553	-2.390301	-0.004407
N35	-2.794385	-1.921566	0.008799
H36	-3.008226	-2.909748	0.015417
O37	-6.407327	0.984163	-0.157819
H38	-5.497727	1.277827	-0.015475
H39	-6.982026	1.556174	0.351481

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C1	2.008077	1.174539	0.000759
C2	1.685181	-0.206656	-0.003014
C3	4.340991	0.365956	-0.006323
C4	0.757152	-2.121412	-0.000252
N5	0.466784	-0.846897	-0.000880
N6	2.104951	-2.357574	-0.003192
N7	4.038378	-0.905839	-0.011575
C8	2.712221	-1.134801	-0.002832
N9	5.636494	0.748971	0.027016
H10	6.323639	0.019506	-0.067143
H11	5.919313	1.686388	-0.199229
O12	1.249121	2.142812	0.008084
H13	0.024937	-2.916660	0.000834
C14	2.779387	-3.646604	0.014735
H15	3.520969	-3.680836	-0.782472
H16	3.273437	-3.798129	0.974662
H17	2.038879	-4.429129	-0.142712
H18	-1.170459	-0.325016	-0.000723
C19	-2.536995	1.251262	-0.004310
C20	-3.927506	1.558083	-0.007828
C21	-4.801727	0.525090	-0.009481
H22	-4.269028	2.581811	-0.010039
H23	-5.871402	0.694305	-0.012007
N24	-2.188602	-0.053838	-0.003589
C25	-3.065131	-1.124161	-0.000306
O26	-2.684117	-2.268555	0.008292
N27	-4.414150	-0.776473	-0.008783
C28	-5.379267	-1.878211	0.004766
H29	-5.173336	-2.555357	-0.822895
H30	-5.300753	-2.430282	0.941294
H31	-6.380328	-1.463781	-0.097868
N32	-1.589723	2.157767	-0.002222
H33	-1.775936	3.154615	-0.000251
H34	-0.591756	1.923846	0.001552
N35	3.394722	1.367337	0.000158
H36	3.688363	2.333710	0.040283
O37	-0.340258	4.585511	0.012013
H38	-0.121901	5.516785	0.038090
H39	0.491102	4.097394	0.017485

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C1	-2.398291	-1.468700	-0.008269
C2	-2.138526	-0.074279	-0.010085
C3	-4.763237	-0.757224	0.007552
C4	-1.281837	1.872456	-0.008627
N5	-0.946483	0.608951	-0.016006
N6	-2.638046	2.057014	0.000679
N7	-4.516122	0.527231	0.003865
C8	-3.199744	0.811383	0.001967
N9	-6.042182	-1.194452	0.052172
H10	-6.758409	-0.493401	-0.040218
H11	-6.285492	-2.140977	-0.182106
O12	-1.601761	-2.402031	-0.010069
H13	-0.578499	2.692894	-0.011223
C14	-3.359612	3.319574	0.028359

H15	-4.107589	3.329762	-0.763585
H16	-3.852529	3.449825	0.992071
H17	-2.649562	4.129529	-0.131051
H18	0.642074	0.028767	-0.019233
C19	2.085358	-1.504167	-0.005735
C20	3.484858	-1.742910	0.003140
C21	4.317560	-0.671334	0.002060
H22	3.877842	-2.748328	0.011487
H23	5.398149	-0.782399	0.009779
N24	1.671173	-0.221824	-0.015500
C25	2.500983	0.888895	-0.017007
O26	2.066484	2.014263	-0.025631
N27	3.863700	0.605709	-0.007512
C28	4.779407	1.750890	-0.011671
H29	4.618629	2.343360	-0.912091
H30	4.584462	2.376288	0.859026
H31	5.799341	1.371655	0.014704
N32	1.186642	-2.472230	-0.004612
H33	1.503287	-3.427474	0.003081
H34	0.166638	-2.316029	-0.009189
N35	-3.777441	-1.718784	0.002002
H36	-4.027301	-2.697747	0.041442
O37	7.502829	-0.374761	0.040763
H38	8.066413	-0.451849	0.813241
H39	8.091934	-0.452453	-0.712366

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C1	-2.091959	-1.603108	0.026942
C2	-1.737547	-0.232485	0.021658
C3	-4.404846	-0.747085	-0.012613
C4	-0.764496	1.663317	0.019960
N5	-0.502259	0.379130	0.034695
N6	-2.105804	1.924311	-0.003409
N7	-4.074069	0.517485	-0.024686
C8	-2.742842	0.717948	0.000008
N9	-5.710093	-1.101446	0.011209
H10	-6.377592	-0.356987	-0.104486
H11	-6.008279	-2.031547	-0.225754
O12	-1.360427	-2.592083	0.044775
H13	-0.036421	2.465519	0.024035
C14	-2.737142	3.234921	-0.015045
H15	-3.457807	3.285536	-0.830534
H16	-3.249361	3.411909	0.930980
H17	-1.962753	3.986250	-0.160977
H18	1.050106	-0.268249	0.042695
C19	2.331913	-1.945257	-0.017177
C20	3.700633	-2.339152	-0.058265
C21	4.642553	-1.370012	-0.051347
H22	3.974769	-3.382580	-0.096525
H23	5.698720	-1.606747	-0.083312
N24	2.058994	-0.623201	0.027548
C25	3.012764	0.377572	0.040267
O26	2.720132	1.549462	0.088832
N27	4.335147	-0.048962	-0.005307
C28	5.368079	0.989885	0.011983
H29	5.211224	1.678707	-0.817060
H30	5.321762	1.543425	0.949605
H31	6.341121	0.512808	-0.086303
N32	1.346428	-2.816433	-0.021505
H33	1.572467	-3.797325	-0.054803
H34	0.336450	-2.575714	0.011184
N35	-3.481815	-1.767866	0.012198
H36	-3.791853	-2.729297	0.054991
O37	1.291968	4.026008	-0.103883
H38	2.025330	3.406940	-0.022049
H39	1.610382	4.869860	0.217088

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C1	-2.204350	-1.538954	-0.007330
C2	-2.077803	-0.125917	-0.011156
C3	-4.626581	-1.055777	0.006516
C4	-1.411692	1.893745	-0.012868
N5	-0.956337	0.668326	-0.017150
N6	-2.779121	1.947986	-0.005818
N7	-4.502147	0.246090	-0.000339
C8	-3.218887	0.654224	-0.002020
N9	-5.858375	-1.611794	0.053469
H10	-6.637488	-0.981227	-0.038427
H11	-6.011922	-2.577487	-0.178669
O12	-1.323083	-2.392582	-0.007405
H13	-0.791319	2.778620	-0.015993
C14	-3.618397	3.135518	0.018554
H15	-4.378673	3.059541	-0.757970
H16	-4.103640	3.234544	0.989907
H17	-2.994749	4.008277	-0.168585
H18	0.680579	0.244804	-0.014925
C19	2.264208	-1.143750	-0.006165
C20	3.679885	-1.248920	0.001083
C21	4.402900	-0.102778	0.005423
H22	4.185130	-2.203085	0.003796
H23	5.485810	-0.147550	0.011568
N24	1.728943	0.093957	-0.009857
C25	2.448435	1.278481	-0.005324
O26	1.910106	2.358406	-0.008146
N27	3.832160	1.127066	0.002738
C28	4.628385	2.355664	0.008144
H29	4.400353	2.946994	-0.878197
H30	4.392844	2.944302	0.894354
H31	5.682351	2.084988	0.012302
N32	1.462216	-2.193190	-0.009412
H33	1.870947	-3.112895	-0.005861
H34	0.432127	-2.136610	-0.011180
N35	-3.553778	-1.919072	0.002837
H36	-3.708861	-2.917337	0.045305
O37	6.857014	-1.951139	0.014934
H38	7.363204	-2.235389	0.778363
H39	7.369467	-2.232775	-0.745280

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C1	-2.182772	-1.448115	0.029075
C2	-1.869423	-0.067068	-0.057735
C3	-4.516884	-0.642753	0.089391

C4	-0.941472	1.840689	-0.200812
N5	-0.653162	0.566904	-0.145117
N6	-2.288773	2.079334	-0.154375
N7	-4.220940	0.628581	0.003658
C8	-2.895736	0.858969	-0.060770
N9	-5.808911	-1.024330	0.203818
H10	-6.501341	-0.301731	0.097300
H11	-6.097332	-1.972645	0.037851
O12	-1.424499	-2.412293	0.047413
H13	-0.209808	2.632231	-0.277679
C14	-2.963235	3.367566	-0.182274
H15	-3.706019	3.375543	-0.979294
H16	-3.456793	3.552076	0.772103
H17	-2.223029	4.144468	-0.366964
H18	0.923755	-0.081966	-0.211468
C19	2.286460	-1.678809	-0.237105
C20	3.670513	-1.987819	-0.321224
C21	4.542420	-0.957775	-0.441558
H22	4.016113	-3.009982	-0.293029
H23	5.609214	-1.130409	-0.511023
N24	1.933627	-0.381518	-0.287627
C25	2.815598	0.684215	-0.346314
O26	2.437998	1.830177	-0.298824
N27	4.154212	0.336034	-0.490599
C28	5.123527	1.431031	-0.497254
H29	4.807249	2.189222	-1.210677
H30	5.181983	1.870644	0.499071
H31	6.094513	1.034303	-0.788299
N32	1.349603	-2.602465	-0.121749
H33	1.623289	-3.570551	-0.097198
H34	0.339824	-2.399248	-0.062988
N35	-3.569325	-1.641640	0.103561
H36	-3.854478	-2.606695	0.202617
O37	3.491364	0.633012	2.375254
H38	3.020784	1.453768	2.534384
H39	3.704874	0.286704	3.243037

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C1	-1.451224	-1.746749	0.068761
C2	-1.280750	-0.340259	0.138147
C3	-3.854764	-1.200033	0.177961
C4	-0.544834	1.650016	0.242163
N5	-0.132158	0.411735	0.153304
N6	-1.907269	1.753984	0.283116
N7	-3.688646	0.098217	0.229612
C8	-2.391159	0.479074	0.215718
N9	-5.105854	-1.712474	0.160010
H10	-5.857919	-1.077350	0.372752
H11	-5.275129	-2.691257	0.314864
O12	-0.597717	-2.623546	-0.009208
H13	0.106451	2.511462	0.279015
C14	-2.683484	2.981990	0.430362
H15	-3.440374	3.042650	-0.351780
H16	-3.169893	2.994214	1.406134
H17	-1.999736	3.826043	0.355509
H18	1.475332	-0.059002	0.063628
C19	3.014246	-1.486664	-0.133238
C20	4.425998	-1.629547	-0.235138
C21	5.181411	-0.505376	-0.199630
H22	4.881557	-2.602328	-0.340754
H23	6.260789	-0.551904	-0.275536
N24	2.520468	-0.240300	-0.003949
C25	3.275356	0.921869	0.035162
O26	2.774071	2.011379	0.151515
N27	4.652954	0.735324	-0.070976
C28	5.484411	1.941057	-0.027546
H29	5.179429	2.625340	-0.818142
H30	5.364538	2.437649	0.934946
H31	6.524298	1.652995	-0.168832
N32	2.184258	-2.511951	-0.160526
H33	2.561412	-3.440242	-0.257662
H34	1.157775	-2.427132	-0.090704
N35	-2.811073	-2.090419	0.104270
H36	-2.995865	-3.082972	0.046125
O37	-5.316175	2.130010	-1.132336
H38	-4.959382	1.324473	-0.735426
H39	-5.734719	1.873541	-1.954269

Cartesian coordinates for the structures in Figure 4, optimized at ωB97XD/ 6-311++ G(d,p).

HG-9MG·[1MC + $H_{N3'}$]$^+$

C1	-1.931107	-1.442366	-0.010694
C2	-1.638144	-0.055147	-0.010444
C3	-4.278253	-0.677256	-0.000014
C4	-0.737374	1.872188	-0.005478
N5	-0.430335	0.601092	-0.013268
N6	-2.088534	2.087400	0.001194
N7	-4.000617	0.601410	-0.000999
C8	-2.678672	0.854920	-0.000007
N9	-5.566188	-1.083732	0.037968
H10	-6.268035	-0.367623	-0.048263
H11	-5.832574	-2.028028	-0.179049
O12	-1.156018	-2.394576	-0.011510
H13	-0.016478	2.677130	-0.006253
C14	-2.781902	3.366019	0.029407
H15	-3.526692	3.394337	-0.765050
H16	-3.275083	3.504250	0.991815
H17	-2.053678	4.160535	-0.125440
H18	1.132254	-0.015499	-0.013828
C19	2.531665	-1.592540	0.006385
C20	3.926580	-1.873955	0.019813
C21	4.785584	-0.827032	0.019140
H22	4.289514	-2.890509	0.031626
H23	5.857734	-0.979767	0.029503
N24	2.156645	-0.298596	-0.006743
C25	3.018959	0.786851	-0.010814
O26	2.621424	1.924408	-0.027356
N27	4.375324	0.464410	0.006714
C28	5.318964	1.585254	-0.006260
H29	5.224882	2.137999	-0.940781
H30	5.102168	2.255270	0.824420
H31	6.328306	1.190160	0.091029
N32	1.609767	-2.535171	0.006756
H33	1.901005	-3.498815	0.016592
H34	0.591852	-2.353101	-0.002346
N35	-3.314579	-1.661376	-0.004394
H36	-3.586596	-2.634662	0.030152

9MG

C1	1.130078	1.404449	0.000953
C2	-0.252707	1.012959	-0.010429
C3	1.530191	-1.060337	0.000920
C4	-2.362999	0.899735	-0.009242
N5	-1.398413	1.772536	-0.011645
N6	-1.921611	-0.405464	-0.008779
N7	0.275565	-1.407026	-0.013323
C8	-0.560681	-0.337519	-0.006196
N9	2.501787	-2.026910	0.060594
H10	2.152331	-2.958101	-0.101169
H11	3.391817	-1.830289	-0.367766
O12	1.649014	2.495475	0.013391
H13	-3.419418	1.128912	-0.010787
C14	-2.715824	-1.615635	0.020462
H15	-2.383535	-2.296716	-0.763527
H16	-2.619839	-2.114348	0.986647
H17	-3.760187	-1.354346	-0.148704
N18	1.956342	0.237907	0.006673
H19	2.942679	0.441882	0.084726

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

H1	1.019516	1.948980	0.000040
C2	1.586902	-0.038189	-0.000003
C3	1.059547	-1.346102	-0.000056
C4	-0.294556	-1.489483	-0.000001
H5	1.708921	-2.208219	-0.000100
H6	-0.748789	-2.472866	-0.000035
N7	0.705663	0.985433	0.000065
C8	-0.694773	0.868738	0.000009
O9	-1.407127	1.826607	-0.000075
N10	-1.151611	-0.448882	0.000096
C11	-2.611549	-0.627244	-0.000014
H12	-3.034998	-0.157781	0.886815
H13	-3.034615	-0.161159	-0.888822
H14	-2.828944	-1.693130	0.002008
N15	2.887659	0.220768	-0.000007
H16	3.553812	-0.535210	-0.000060
H17	3.256715	1.158969	0.000059

TS_PT3′

C1	-1.933338	-1.484865	-0.007187
C2	-1.580277	-0.106757	-0.004940
C3	-4.243355	-0.598859	0.002770
C4	-0.591979	1.809427	-0.007015
N5	-0.354321	0.517602	-0.009684
N6	-1.922719	2.063954	-0.001871
N7	-3.899195	0.667108	0.005264
C8	-2.570000	0.852424	0.000696
N9	-5.546066	-0.931522	0.005981
H10	-6.220414	-0.185130	0.011189
H11	-5.872837	-1.880927	0.004667
O12	-1.204821	-2.463725	-0.011878
H13	0.184043	2.560428	-0.010007
C14	-2.568532	3.370166	0.019252
H15	-3.300114	3.423828	-0.785668
H16	-3.069132	3.519528	0.975625
H17	-1.808922	4.136782	-0.122545
H18	0.763172	0.023410	-0.011813
C19	2.523133	-1.619276	0.003094
C20	3.932138	-1.842487	0.015847
C21	4.735625	-0.754143	0.016434
H22	4.346418	-2.839672	0.025586
H23	5.814908	-0.843617	0.026197
N24	2.047863	-0.369441	-0.008232
C25	2.865076	0.733625	-0.008990
O26	2.422415	1.867621	-0.020980
N27	4.243330	0.507977	0.005593
C28	5.113235	1.683870	-0.000627

H29	4.953902	2.257821	-0.913200
H30	4.883905	2.316427	0.856093
H31	6.148966	1.352696	0.051747
N32	1.665138	-2.635306	0.002591
H33	2.012971	-3.578642	0.011035
H34	0.651778	-2.502467	-0.005931
N35	-3.329865	-1.629142	-0.002809
H36	-3.648909	-2.589008	-0.003931

HG-[9MG + H_{N7}]$^+$·1MC

C1	-1.927032	-1.493369	-0.004072
C2	-1.602540	-0.105503	-0.003303
C3	-4.251501	-0.635894	0.002855
C4	-0.638193	1.839850	-0.007520
N5	-0.394384	0.547671	-0.007942
N6	-1.969314	2.065507	-0.003858
N7	-3.925935	0.636725	0.003658
C8	-2.601079	0.840975	0.000032
N9	-5.548506	-0.985119	0.005539
H10	-6.232983	-0.247761	0.009047
H11	-5.863027	-1.938848	0.005423
O12	-1.180810	-2.453724	-0.007158
H13	0.137063	2.591660	-0.010631
C14	-2.638699	3.361323	0.013394
H15	-3.369380	3.398139	-0.793063
H16	-3.143039	3.501624	0.968951
H17	-1.892327	4.140584	-0.128788
H18	0.601232	0.094372	-0.010218
C19	2.612949	-1.630162	0.000825
C20	4.030048	-1.806433	0.010380
C21	4.789229	-0.686567	0.011521
H22	4.483524	-2.786576	0.016984
H23	5.871413	-0.730216	0.018829
N24	2.081632	-0.409940	-0.007099
C25	2.854261	0.716103	-0.006072
O26	2.368143	1.838215	-0.013238
N27	4.243203	0.553922	0.004062
C28	5.062636	1.763996	0.002535
H29	4.859719	2.347822	-0.895019
H30	4.826265	2.371890	0.875400
H31	6.112785	1.477276	0.026484
N32	1.789058	-2.681339	-0.000166
H33	2.160389	-3.615026	0.005939
H34	0.778467	-2.563923	-0.005612
N35	-3.324031	-1.653872	-0.000416
H36	-3.631291	-2.617745	-0.000451

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

C1	1.153387	1.398786	0.001852
C2	-0.217631	0.964019	0.000834
C3	1.581210	-1.052177	-0.000743
C4	-2.404023	0.785343	-0.004237
N5	-1.406538	1.659251	-0.001366
N6	-1.909182	-0.457421	-0.004626
N7	0.311534	-1.411732	-0.000983
C8	-0.526600	-0.372952	-0.000628
N9	2.526371	-1.999300	-0.002373
H10	2.230142	-2.961391	-0.003693
H11	3.510630	-1.795979	-0.003168
O12	1.585459	2.520555	0.002967
H13	-3.453385	1.033005	-0.006545
C14	-2.668552	-1.707067	0.006782
H15	-2.322258	-2.336778	-0.810936
H16	-2.507164	-2.217000	0.955537
H17	-3.725100	-1.479851	-0.121220
H18	-1.500825	2.666100	-0.003010
N19	1.991770	0.259455	0.001338
H20	2.979865	0.479973	0.002191

1MC

C1	-1.536977	-0.033495	0.002257
C2	-1.076252	1.322992	0.001068
C3	0.265977	1.493961	-0.000483
H4	-1.751207	2.166725	0.008661
H5	0.723004	2.476723	-0.000478
N6	-0.733676	-1.069031	-0.001581
C7	0.620814	-0.898799	0.000283
O8	1.430823	-1.802102	-0.000464
N9	1.110749	0.440485	-0.000410
C10	2.555970	0.612484	-0.001696
H11	2.989249	0.139041	0.879877
H12	2.987771	0.140913	-0.885030
H13	2.786087	1.678197	-0.000708
N14	-2.870707	-0.282567	0.028971
H15	-3.538650	0.449909	-0.126031
H16	-3.164592	-1.239747	-0.070019

TS_PT7

C1	-1.421056	-1.325068	-0.015381
C2	-1.503186	0.113414	-0.013318
C3	-3.911277	-1.196145	0.002832
C4	-1.232486	2.254278	-0.008709
N5	-0.560193	1.128487	-0.017579
N6	-2.568789	2.050173	0.000092
N7	-3.973138	0.111400	0.003353
C8	-2.762692	0.693690	-0.000932
N9	-5.048295	-1.919106	0.033388
H10	-5.917489	-1.415824	-0.023247
H11	-5.061256	-2.913045	-0.109957
O12	-0.473419	-2.080814	-0.020808
H13	-0.782715	3.235445	-0.009290
C14	-3.622013	3.054750	0.029414
H15	-4.328785	2.861982	-0.776465
H16	-4.144802	3.015800	0.984862
H17	-3.171687	4.036898	-0.104398
H18	0.721575	1.253365	-0.022240
C19	2.983484	-1.647284	0.008401
C20	4.401615	-1.463746	0.019565
C21	4.850083	-0.187736	0.015910
H22	5.094338	-2.293078	0.030349
H23	5.904973	0.054412	0.023870
N24	2.161907	-0.602214	-0.004708

C25	2.641876	0.624138	-0.008207
O26	1.858948	1.624939	-0.021035
N27	3.995140	0.873745	0.002161
C28	4.471739	2.257868	-0.001706
H29	4.119012	2.768326	-0.897175
H30	4.096499	2.780477	0.877419
H31	5.560152	2.251362	0.012350
N32	2.409016	-2.848497	0.010485
H33	2.946074	-3.697142	0.019180
H34	1.394068	-2.872502	0.000623
N35	-2.724979	-1.879442	-0.006316
H36	-2.725379	-2.890243	0.015506

HG-9MG·[1MC + H$_{O2'}$]$^+$

C1	-1.428515	-1.295894	-0.018555
C2	-1.527477	0.138123	-0.016885
C3	-3.917559	-1.208515	0.003174
C4	-1.278335	2.265406	-0.010215
N5	-0.586437	1.154911	-0.022051
N6	-2.621152	2.052986	0.001352
N7	-4.001396	0.095483	0.003147
C8	-2.798290	0.698511	-0.000776
N9	-5.043465	-1.955888	0.047718
H10	-5.915533	-1.461479	-0.041213
H11	-5.037226	-2.933580	-0.184369
O12	-0.468459	-2.043069	-0.023633
H13	-0.853224	3.258393	-0.010778
C14	-3.681337	3.047794	0.035383
H15	-4.392826	2.849946	-0.765410
H16	-4.199166	3.009607	0.993886
H17	-3.239792	4.033416	-0.103660
H18	0.952956	1.367858	-0.027602
C19	2.954243	-1.647623	0.009905
C20	4.377674	-1.510583	0.023666
C21	4.872260	-0.251854	0.019288
H22	5.041486	-2.363355	0.036722
H23	5.934654	-0.046328	0.028970
N24	2.173066	-0.565647	-0.006005
C25	2.705085	0.625841	-0.009510
O26	1.953547	1.674618	-0.024720
N27	4.055071	0.841831	0.002679
C28	4.581315	2.210373	-0.002141
H29	4.248149	2.731407	-0.898835
H30	4.226903	2.745601	0.877873
H31	5.668358	2.161903	0.011466
N32	2.329777	-2.817607	0.011865
H33	2.829274	-3.689389	0.023409
H34	1.311139	-2.792701	0.000476
N35	-2.720386	-1.873194	-0.007565
H36	-2.705804	-2.883298	0.027904

[1MC + H$_{O2'}$]$^+$

H1	-1.006457	2.585579	0.000027
C2	1.580136	0.014747	0.000007
C3	1.116731	-1.333627	0.000059
C4	-0.220685	-1.529939	0.000023
H5	1.797731	-2.172889	0.000095
H6	-0.666480	-2.515625	0.000035
N7	0.708089	1.036979	0.000003
C8	-0.567762	0.768610	0.000004
O9	-1.458002	1.731524	0.000044
N10	-1.094197	-0.480105	-0.000045
C11	-2.553944	-0.679729	-0.000030
H12	-2.986501	-0.227107	0.890879
H13	-2.986747	-0.224883	-0.889673
H14	-2.749591	-1.749529	-0.001381
N15	2.871515	0.317387	-0.000041
H16	3.583826	-0.393745	-0.000043
H17	3.153534	1.285807	-0.000087

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

HG-9MG·[1MC + $H_{N3'}$]$^+$·H_2O

C1	-1.777697	-0.937746	-0.005328
C2	-1.278442	0.390486	-0.005302
C3	-3.978472	0.163172	0.002102
C4	-0.102620	2.165701	-0.007921
N5	0.013760	0.863260	-0.009586
N6	-1.407014	2.577187	-0.004449
N7	-3.516124	1.392247	0.003203
C8	-2.173796	1.444468	-0.001130
N9	-5.304190	-0.060244	0.005008
H10	-5.914301	0.738092	0.008417
H11	-5.678136	-0.997803	0.004416
O12	-1.143207	-1.993346	-0.007765
H13	0.727777	2.857017	-0.010767
C14	-1.907602	3.941843	0.017940
H15	-2.634177	4.077032	-0.782683
H16	-2.385912	4.149854	0.975425
H17	-1.072456	4.624967	-0.129193
H18	1.454378	0.036964	-0.010075
C19	2.604034	-1.733772	0.002541
C20	3.940983	-2.224669	0.011456
C21	4.948572	-1.320475	0.010996
H22	4.143715	-3.284846	0.018803
H23	5.985408	-1.633482	0.017726
N24	2.428935	-0.398068	-0.006172
C25	3.445798	0.542832	-0.006058
O26	3.228461	1.728426	-0.012801
N27	4.738145	0.018226	0.002461
C28	5.839205	0.983866	0.001561
H29	5.781820	1.608146	-0.889548
H30	5.772357	1.620801	0.882966
H31	6.781039	0.438605	0.010504
N32	1.550265	-2.525535	0.002556
H33	1.694560	-3.521781	0.009304
H34	0.567229	-2.193488	-0.003234
N35	-3.171487	-0.953200	-0.001526
H36	-3.617140	-1.869143	-0.001163
O37	-5.257824	-3.033611	-0.000028
H38	-5.454630	-3.578608	0.765393
H39	-5.456778	-3.575422	-0.767156

H_2O

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

TS_PT3′·H_2O

C1	-1.785083	-0.976575	-0.004129
C2	-1.225724	0.332430	-0.001548
C3	-3.928120	0.241407	0.001946
C4	0.038644	2.078019	-0.002182
N5	0.081027	0.765617	-0.004614
N6	-1.238938	2.530473	0.001345
N7	-3.401961	1.447263	0.005373
C8	-2.061633	1.429437	0.002713
N9	-5.261130	0.087928	0.003056
H10	-5.830270	0.916307	0.005936
H11	-5.682616	-0.829855	-0.000968
O12	-1.201149	-2.052903	-0.007317
H13	0.917559	2.705708	-0.004517
C14	-1.683183	3.917042	0.021266
H15	-2.384281	4.084362	-0.795397
H16	-2.174995	4.133825	0.969372
H17	-0.816200	4.564041	-0.100164
H18	1.131916	0.104130	-0.006445
C19	2.585731	-1.776007	0.009232
C20	3.941025	-2.223692	0.019100
C21	4.909913	-1.280227	0.013590
H22	4.186398	-3.275205	0.030999
H23	5.960796	-1.542221	0.020076
N24	2.321304	-0.464712	-0.003991
C25	3.305665	0.492855	-0.010212
O26	3.053110	1.682664	-0.023646
N27	4.629114	0.045193	0.000141
C28	5.678713	1.063323	-0.014512
H29	5.613029	1.651566	-0.929658
H30	5.559251	1.729699	0.838955
H31	6.646622	0.567739	0.037175
N32	1.575161	-2.638391	0.013191
H33	1.768506	-3.625035	0.022407
H34	0.592397	-2.346003	0.004158
N35	-3.179467	-0.914108	-0.002350
H36	-3.673489	-1.806004	-0.004699
O37	-5.352717	-2.880156	-0.012822
H38	-5.571177	-3.421617	0.749449
H39	-5.568848	-3.411187	-0.783061

HG-[9MG + H_{N7}]$^+$ ·1MC·H_2O

C1	-1.782766	-0.984579	-0.006760
C2	-1.253956	0.340897	-0.005185
C3	-3.946962	0.203690	0.005124
C4	-0.012329	2.125139	-0.008075
N5	0.037013	0.811089	-0.011089
N6	-1.295421	2.543657	-0.001437
N7	-3.440767	1.420330	0.007429
C8	-2.102297	1.424723	0.001450
N9	-5.275917	0.030569	0.009670
H10	-5.858178	0.849995	0.014238
H11	-5.683413	-0.893877	0.006671
O12	-1.175996	-2.042513	-0.011762
H13	0.866047	2.753533	-0.011583
C14	-1.770104	3.921663	0.019973
H15	-2.477009	4.070746	-0.794941
H16	-2.264103	4.124362	0.969792
H17	-0.918329	4.587912	-0.103500
H18	0.949256	0.220173	-0.014226
C19	2.682742	-1.798486	0.004738

C20	4.055063	-2.196073	0.018641
C21	4.981044	-1.210177	0.018453
H22	4.347562	-3.235708	0.030157
H23	6.043108	-1.422327	0.028934
N24	2.350241	-0.510549	-0.008386
C25	3.289729	0.479671	-0.010125
O26	2.987594	1.664496	-0.024441
N27	4.636922	0.100840	0.006265
C28	5.637457	1.165433	-0.004225
H29	5.561699	1.739397	-0.927904
H30	5.471313	1.836640	0.837579
H31	6.626690	0.716702	0.071430
N32	1.703652	-2.706710	0.005061
H33	1.924144	-3.686856	0.014161
H34	0.722965	-2.430910	-0.004206
N35	-3.180267	-0.940014	-0.001311
H36	-3.662306	-1.839097	-0.002587
O37	-5.314430	-2.936060	-0.006473
H38	-5.519470	-3.482345	0.756224
H39	-5.521231	-3.471608	-0.776285

TS_PT7·H_2O

C1	-1.342335	-0.823438	-0.005369
C2	-1.185283	0.609870	-0.004392
C3	-3.770274	-0.294137	0.004896
C4	-0.570960	2.676069	-0.008820
N5	-0.087488	1.458042	-0.010254
N6	-1.924138	2.693349	-0.003905
N7	-3.623942	1.010214	0.006308
C8	-2.336078	1.386239	0.000815
N9	-4.999109	-0.837530	0.009021
H10	-5.787829	-0.215057	0.012502
H11	-5.128348	-1.838815	0.005762
O12	-0.520949	-1.720858	-0.009984
H13	0.027533	3.574635	-0.012583
C14	-2.800152	3.853939	0.016247
H15	-3.545264	3.758195	-0.772393
H16	-3.304841	3.924705	0.979877
H17	-2.202650	4.748702	-0.151795
H18	1.254042	1.389061	-0.013235
C19	2.934525	-1.857194	0.005100
C20	4.363661	-1.921300	0.012044
C21	5.025527	-0.741732	0.009974
H22	4.901872	-2.858360	0.018781
H23	6.106329	-0.683788	0.014888
N24	2.308118	-0.684167	-0.002871
C25	2.992837	0.436249	-0.004803
O26	2.393045	1.561371	-0.012785
N27	4.367032	0.452362	0.001801
C28	5.075461	1.733544	-0.002140
H29	4.818991	2.295838	-0.899443
H30	4.793944	2.314588	0.875369
H31	6.146285	1.539085	0.015346
N32	2.156274	-2.936016	0.006063
H33	2.534521	-3.866345	0.011565
H34	1.151713	-2.773936	0.000367
N35	-2.710110	-1.160923	-0.000062
H36	-2.907396	-2.159267	-0.000924
O37	-4.243273	-3.704047	-0.007685
H38	-4.308107	-4.284609	0.754012
H39	-4.309401	-4.272330	-0.778492

HG-9MG·[1MC + $H_{O2'}$]$^+$·H_2O

C1	-1.343645	-0.807424	-0.011459
C2	-1.200072	0.625001	-0.008672
C3	-3.776490	-0.308915	0.009548
C4	-0.604912	2.686881	-0.011867
N5	-0.105345	1.477244	-0.017762
N6	-1.962858	2.696439	-0.001104
N7	-3.645878	0.996043	0.013024
C8	-2.361411	1.387895	0.002884
N9	-4.999399	-0.868122	0.018189
H10	-5.795311	-0.255076	0.023753
H11	-5.116590	-1.870624	0.009628
O12	-0.512453	-1.699567	-0.020951
H13	-0.022509	3.596564	-0.016631
C14	-2.846689	3.849755	0.025289
H15	-3.594730	3.752178	-0.760563
H16	-3.348577	3.916506	0.990874
H17	-2.256339	4.749349	-0.143107
H18	1.398182	1.440901	-0.025150
C19	2.918938	-1.846112	0.011673
C20	4.346586	-1.936897	0.023939
C21	5.032888	-0.771371	0.018582
H22	4.866519	-2.884198	0.037154
H23	6.114485	-0.735207	0.026891
N24	2.318980	-0.655746	-0.003538
C25	3.029864	0.439642	-0.008594
O26	2.452498	1.589548	-0.024681
N27	4.398914	0.437348	0.002753
C28	5.133879	1.705058	-0.008633
H29	4.908359	2.255758	-0.921302
H30	4.846598	2.306050	0.853180
H31	6.199508	1.488462	0.035369
N32	2.114854	-2.901720	0.014267
H33	2.469275	-3.841629	0.024232
H34	1.112748	-2.710568	0.002970
N35	-2.705899	-1.163177	-0.001462
H36	-2.890635	-2.163570	-0.003982
O37	-4.215054	-3.728518	-0.017717
H38	-4.277930	-4.314896	0.739579
H39	-4.280198	-4.290935	-0.792815

TS1

C1	2.469365	-1.375298	0.013790
C2	2.037795	-0.022571	0.016082
C3	4.729409	-0.376023	0.014320
C4	0.949386	1.802668	0.011507
N5	0.770251	0.508468	0.013981
N6	2.273399	2.153445	0.013014
N7	4.324857	0.867388	0.019880
C8	2.982924	0.986096	0.013398

N9	6.053759	-0.650808	-0.026074
H10	6.675498	0.134227	0.075457
H11	6.410344	-1.557548	0.220824
O12	1.797710	-2.400577	0.008871
H13	0.152635	2.532507	0.010720
C14	2.837727	3.493028	-0.008774
H15	3.570875	3.593682	0.790914
H16	3.323057	3.680666	-0.966968
H17	2.035501	4.213944	0.141158
H18	-0.779620	-0.266729	0.007352
C19	-1.998771	-1.972249	-0.008382
C20	-3.350427	-2.394244	-0.032949
C21	-4.309237	-1.422312	-0.026842
H22	-3.604055	-3.444006	-0.042361
H23	-5.360113	-1.698177	-0.035169
N24	-1.760288	-0.644632	0.004833
C25	-2.752751	0.330991	-0.007243
O26	-2.447097	1.513866	-0.038174
N27	-4.055297	-0.100882	0.010817
C28	-5.237379	1.572337	-1.144977
H29	-6.153252	2.128520	-1.027983
H30	-4.281807	2.072674	-1.023788
H31	-5.282631	0.689914	-1.764997
N32	-0.975470	-2.812911	-0.002490
H33	-1.161185	-3.801574	-0.013952
H34	0.012034	-2.522795	0.006992
N35	3.870543	-1.451711	0.011749
H36	4.239683	-2.392028	-0.030904
O37	-5.918647	1.473349	0.988331
H38	-5.165811	0.868712	1.108286
H39	-5.747394	2.261873	1.512649

HG-9MG· [1HC + $H_{N3'}$]$^+$

C1	-1.515359	-1.468647	-0.005751
C2	-1.334012	-0.062813	-0.008362
C3	-3.915624	-0.893447	0.001647
C4	-0.589678	1.930263	-0.008703
N5	-0.182341	0.687433	-0.011824
N6	-1.953231	2.037200	-0.004727
N7	-3.740638	0.403312	-0.003357
C8	-2.443651	0.761555	-0.002132
N9	-5.166715	-1.400614	0.040342
H10	-5.923447	-0.742464	-0.043755
H11	-5.358679	-2.365093	-0.165945
O12	-0.665201	-2.355357	-0.004428
H13	0.064715	2.790247	-0.010695
C14	-2.745742	3.257271	0.017253
H15	-3.501684	3.213776	-0.765837
H16	-3.234285	3.370961	0.985221
H17	-2.085992	4.104898	-0.161045
H18	1.407909	0.191049	-0.010052
C19	2.938637	-1.266089	0.001106
C20	4.356999	-1.444671	0.009043
C21	5.133635	-0.339138	0.010451
H22	4.790171	-2.433324	0.014318
H23	6.214925	-0.392649	0.016832
N24	2.455108	-0.007582	-0.005514
C25	3.226831	1.145621	-0.003812
O26	2.752615	2.250368	-0.008813
N27	4.595649	0.906456	0.004242
N28	2.098247	-2.279545	0.000140
H29	2.466872	-3.216718	0.005571
H30	1.067290	-2.181077	-0.003524
N31	-2.876219	-1.797893	0.000400
H32	-3.069610	-2.789772	0.036870
H33	5.181275	1.729279	0.005619

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

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

H1	-0.110859	-1.970930	0.000105
C2	-1.189551	-0.208415	0.000000
C3	-1.046724	1.201662	-0.000082
C4	0.209887	1.714206	-0.000013
H5	-1.912983	1.845615	-0.000168
H6	0.392747	2.781694	-0.000034
N7	-0.065652	-0.958299	0.000109
C8	1.254533	-0.466223	0.000006
O9	2.204654	-1.183070	-0.000129
N10	1.304810	0.922534	0.000118
N11	-2.370599	-0.805982	-0.000002
H12	-3.216142	-0.257133	-0.000075
H13	-2.474631	-1.809309	0.000047
H14	2.235858	1.319477	0.000110

TS1_PT3′

C1	-1.521204	-1.513611	0.000036
C2	-1.287704	-0.111067	0.000410
C3	-3.897837	-0.829645	-0.000182
C4	-0.466004	1.880728	-0.004138
N5	-0.118941	0.614049	-0.002004
N6	-1.813946	2.022189	-0.004528
N7	-3.664223	0.461286	-0.000037
C8	-2.355929	0.760278	-0.000274
N9	-5.166769	-1.274106	-0.000795
H10	-5.902899	-0.588520	0.000449
H11	-5.410348	-2.248169	0.000483
O12	-0.709215	-2.425744	-0.000487
H13	0.243223	2.695499	-0.006530
C14	-2.567644	3.269552	0.009142
H15	-3.307585	3.252186	-0.789659
H16	-3.070971	3.387948	0.968431
H17	-1.876081	4.095187	-0.148519
H18	1.050359	0.212386	-0.002806
C19	2.923431	-1.270188	0.000454
C20	4.351465	-1.389484	0.003396

C21	5.070971	-0.247345	0.003460
H22	4.832702	-2.356020	0.005630
H23	6.153510	-0.237443	0.005765
N24	2.345979	-0.062456	-0.002317
C25	3.072418	1.104655	-0.002240
O26	2.554270	2.202239	-0.004550
N27	4.456158	0.961291	0.000738
N28	2.152124	-2.350257	0.000541
H29	2.575240	-3.262737	0.002878
H30	1.129571	-2.301417	-0.000785
N31	-2.899044	-1.778094	0.000323
H32	-3.134666	-2.761762	0.000322
H33	4.986364	1.820349	0.000791

HG-[9MG + H_{N7}]$^{+}$·1HC

C1	-1.517615	-1.520407	0.000157
C2	-1.316864	-0.109500	0.000671
C3	-3.907617	-0.869326	0.000044
C4	-0.524620	1.912807	-0.004398
N5	-0.170791	0.646224	-0.002029
N6	-1.870040	2.021846	-0.004443
N7	-3.695220	0.427136	0.000269
C8	-2.393560	0.746774	0.000017
N9	-5.168624	-1.331850	-0.000523
H10	-5.915417	-0.657571	0.000597
H11	-5.397782	-2.309678	-0.000511
O12	-0.687946	-2.410053	-0.000525
H13	0.184333	2.727889	-0.006937
C14	-2.649680	3.254868	0.008533
H15	-3.388270	3.219699	-0.790721
H16	-3.155155	3.360566	0.967940
H17	-1.975414	4.094511	-0.149041
H18	0.854740	0.280229	-0.003204
C19	3.022474	-1.265338	0.000163
C20	4.455686	-1.328923	0.003398
C21	5.121467	-0.154461	0.003758
H22	4.980776	-2.272580	0.005605
H23	6.202221	-0.091507	0.006302
N24	2.383029	-0.097443	-0.002635
C25	3.056440	1.091653	-0.002179
O26	2.489504	2.171986	-0.004392
N27	4.447711	1.022771	0.001084
N28	2.294389	-2.382862	0.000009
H29	2.743889	-3.281800	0.002396
H30	1.276892	-2.352164	-0.001353
N31	-2.894507	-1.802776	0.000470
H32	-3.116669	-2.789780	0.000467
H33	4.935081	1.906518	0.001400

1HC

C1	1.182095	-0.526650	-0.000084
N2	-0.082021	-1.047475	-0.000685
C3	-1.125659	-0.253079	0.000556
C4	0.202000	1.705764	-0.000320
N5	1.277902	0.888358	-0.000375
H6	0.396535	2.771386	-0.000437
O7	2.206651	-1.172263	-0.000093
N8	-2.346150	-0.837635	0.007967
H9	-2.389356	-1.842139	-0.018633
H10	-3.192401	-0.301154	-0.031945
C11	-1.043632	1.183690	0.000142
H12	-1.921519	1.813417	0.002148
H13	2.216585	1.255509	-0.000506

TS1_PT7

C1	-1.047162	-1.290970	-0.007535
C2	-1.272702	0.131706	-0.003616
C3	-3.537138	-1.413958	0.003496
C4	-1.218586	2.286856	-0.008429
N5	-0.435049	1.235794	-0.009365
N6	-2.528675	1.950215	-0.003971
N7	-3.730758	-0.119818	0.009574
C8	-2.585028	0.581776	0.000527
N9	-4.595683	-2.248642	-0.018599
H10	-5.509717	-1.834995	0.055582
H11	-4.506520	-3.238207	0.128078
O12	-0.027843	-1.948699	-0.015891
H13	-0.872443	3.309459	-0.011918
C14	-3.677814	2.843726	0.014870
H15	-4.358827	2.574329	-0.791189
H16	-4.197059	2.759665	0.969372
H17	-3.328799	3.865379	-0.125916
H18	0.859042	1.502048	-0.010249
C19	3.368045	-1.190067	0.004315
C20	4.768178	-0.873739	0.010140
C21	5.094736	0.436718	0.008840
H22	5.531583	-1.638219	0.015104
H23	6.115959	0.793946	0.012754
N24	2.441660	-0.233178	-0.001028
C25	2.798161	1.031442	-0.002505
O26	1.933035	1.961434	-0.008384
N27	4.120736	1.391035	0.002296
N28	2.913812	-2.438449	0.003973
H29	3.529171	-3.232671	0.006231
H30	1.904505	-2.557797	-0.002616
N31	-2.287924	-1.974215	-0.003240
H32	-2.186933	-2.979791	-0.030076
H33	4.347524	2.374845	0.000940

HG-9MG·[1HC + $H_{O2'}$]$^{+}$

C1	-1.049931	-1.270708	-0.012575
C2	-1.286180	0.147766	-0.012303
C3	-3.536147	-1.422328	0.000069
C4	-1.245843	2.291245	-0.006186
N5	-0.449490	1.252564	-0.014851
N6	-2.560257	1.948803	0.000784
N7	-3.744517	-0.132246	-0.000859
C8	-2.605221	0.583144	-0.001133
N9	-4.585392	-2.273162	0.039618
H10	-5.500825	-1.864596	-0.048588
H11	-4.485687	-3.248694	-0.179438
O12	-0.022702	-1.922582	-0.013493

H13	-0.918733	3.320712	-0.006016
C14	-3.712994	2.835489	0.030010
H15	-4.399530	2.566019	-0.771538
H16	-4.226165	2.748687	0.987785
H17	-3.370387	3.859404	-0.111285
H18	1.028897	1.604754	-0.021147
C19	3.347721	-1.197194	0.008769
C20	4.755607	-0.917872	0.017202
C21	5.120526	0.382533	0.011291
H22	5.498213	-1.702661	0.027654
H23	6.151476	0.710059	0.016689
N24	2.450223	-0.207343	-0.003991
C25	2.850384	1.034083	-0.009106
O26	2.008743	2.004565	-0.021041
N27	4.173933	1.366044	-0.002055
N28	2.850033	-2.424466	0.012789
H29	3.436577	-3.240602	0.021790
H30	1.833717	-2.504173	0.005166
N31	-2.280644	-1.969045	-0.006232
H32	-2.169298	-2.973128	0.028792
H33	4.428677	2.343366	-0.006252

[1HC + $H_{O2'}$]$^+$

H1	-2.089659	-1.968411	0.000569
C2	1.174634	-0.276084	0.000006
C3	1.132634	1.154224	0.000002
C4	-0.083806	1.739396	0.000000
H5	2.034558	1.749616	-0.000018
H6	-0.234790	2.810440	0.000021
N7	0.043146	-1.007945	-0.000002
C8	-1.096603	-0.380217	-0.000004
O9	-2.240097	-1.013839	-0.000089
N10	-1.209623	0.967405	0.000024
N11	2.319158	-0.940379	0.000000
H12	3.209072	-0.469059	-0.000007
H13	2.305499	-1.949562	-0.000068
H14	-2.133829	1.380201	0.000034

TS2

C1	-1.477136	-1.910796	-0.016218
C2	-1.341216	-0.503290	-0.055604
C3	-3.893666	-1.414520	0.028274
C4	-0.697014	1.518397	-0.100654
N5	-0.218856	0.288702	-0.102952
N6	-2.056334	1.597905	-0.036755
N7	-3.762823	-0.117378	-0.007958
C8	-2.469464	0.301867	-0.022199
N9	-5.129383	-1.974870	0.111732
H10	-5.904223	-1.339580	0.016899
H11	-5.283823	-2.921072	-0.192284
O12	-0.602956	-2.777287	-0.010387
H13	-0.054444	2.387917	-0.130559
C14	-3.685967	2.927041	-1.034909
H15	-4.263529	2.031347	-0.835156
H16	-4.170858	3.880814	-0.903718
H17	-2.880010	2.867238	-1.749581
H18	1.350771	-0.097778	-0.084375
C19	2.940843	-1.499201	0.041436
C20	4.358776	-1.619962	0.112861
C21	5.093403	-0.483488	0.091613
H22	4.831894	-2.587432	0.185629
H23	6.174766	-0.510660	0.145531
N24	2.418669	-0.261434	-0.047627
C25	3.153466	0.911514	-0.070083
O26	2.636661	1.998468	-0.147890
N27	4.537808	0.749554	0.004736
C28	5.345221	1.970291	-0.025336
H29	5.206289	2.483124	-0.976870
H30	5.036900	2.634703	0.780822
H31	6.392060	1.699860	0.099647
N32	2.137013	-2.544427	0.059421
H33	2.541693	-3.463465	0.129341
H34	1.102787	-2.491918	0.016134
N35	-2.826868	-2.283863	0.031125
H36	-2.987472	-3.277898	0.120024
O37	-3.412722	3.546214	1.061397
H38	-2.754300	2.827668	1.106582
H39	-2.964434	4.371533	1.269823

HG-9HG·[1MC + $H_{N3'}$]$^+$

C1	-2.167469	1.101560	0.009685
C2	-1.788859	-0.265856	0.008087
C3	-4.462369	0.192620	-0.004542
C4	-0.755503	-2.130156	0.001356
N5	-0.538430	-0.843249	0.010122
N6	-2.092994	-2.423221	-0.006577
N7	-4.104788	-1.066965	-0.003989
C8	-2.772019	-1.237028	-0.002834
N9	-5.771737	0.514053	-0.039227
H10	-6.430138	-0.243937	0.028888
H11	-6.102914	1.446287	0.135045
O12	-1.452557	2.098943	0.012874
H13	0.016269	-2.885316	0.000387
H14	0.988374	-0.109296	0.010386
C15	2.279861	1.555139	-0.000605
C16	3.653545	1.925818	-0.009950
C17	4.578493	0.936591	-0.013556
H18	3.948835	2.964050	-0.015290
H19	5.638676	1.157774	-0.021025
N20	1.989206	0.239253	0.004724
C21	2.920308	-0.788550	0.004563
O22	2.596849	-1.949204	0.014545
N23	4.252500	-0.378622	-0.008949
C24	5.266971	-1.435979	-0.001318
H25	5.204399	-2.002877	0.927327
H26	5.098829	-2.110581	-0.839566
H27	6.248974	-0.975278	-0.088942
N28	1.298917	2.436086	0.002701
H29	1.526566	3.416771	-0.001375
H30	0.295863	2.186685	0.008230
N31	-3.561631	1.234711	0.002746
H32	-3.893100	2.189683	-0.024777

H33	-2.510019	-3.341162	-0.014799

9HG

C1	-0.214456	1.465217	0.002979
C2	0.851208	0.500129	0.008533
C3	-1.664190	-0.566008	-0.003477
C4	2.704126	-0.525479	0.000789
N5	2.216413	0.678757	0.008193
N6	1.726507	-1.496818	-0.004192
N7	-0.693379	-1.433826	0.006510
C8	0.528968	-0.845848	-0.000297
N9	-2.962528	-1.001285	-0.062101
H10	-3.065027	-1.991322	0.094689
H11	-3.675459	-0.428924	0.359929
O12	-0.192783	2.672759	-0.003369
H13	3.754117	-0.777742	-0.001335
N14	-1.471470	0.786868	-0.004051
H15	-2.265468	1.407327	-0.076555
H16	1.851361	-2.495349	-0.011455

TS2_PT3′

C1	-2.159420	1.151336	0.004005
C2	-1.721547	-0.204048	0.002459
C3	-4.409341	0.121870	-0.003580
C4	-0.600355	-2.054292	0.002189
N5	-0.456683	-0.751289	0.004789
N6	-1.915168	-2.382690	-0.001749
N7	-3.985740	-1.120945	-0.004811
C8	-2.650431	-1.221852	-0.001639
N9	-5.729205	0.369546	-0.006861
H10	-6.354075	-0.419072	-0.009308
H11	-6.116657	1.296017	-0.004505
O12	-1.492186	2.171283	0.007562
H13	0.226150	-2.749158	0.003217
H14	0.600612	-0.190576	0.005916
C15	2.288717	1.578707	0.000691
C16	3.681794	1.886119	-0.005481
C17	4.548469	0.847650	-0.009167
H18	4.035851	2.906358	-0.008272
H19	5.620711	0.999821	-0.014465
N20	1.886051	0.304286	0.003688
C21	2.768178	-0.746347	0.002997
O22	2.393201	-1.905744	0.010009
N23	4.130970	-0.441323	-0.007149
C24	5.069187	-1.563578	-0.001978
H25	4.955798	-2.138539	0.916929
H26	4.867602	-2.215643	-0.850852
H27	6.082284	-1.171024	-0.070162
N28	1.372490	2.543697	0.003278
H29	1.662854	3.506207	0.001201
H30	0.370619	2.348423	0.006690
N31	-3.562154	1.207514	0.000664
H32	-3.940785	2.145639	0.001414
H33	-2.294514	-3.317747	-0.004292

HG-[9HG + H_{N7}]$^+$·1MC

C1	-2.158050	1.156165	0.001479
C2	-1.739650	-0.207281	0.000764
C3	-4.419168	0.145123	-0.001104
C4	-0.632587	-2.078421	0.000399
N5	-0.485730	-0.774834	0.001474
N6	-1.948891	-2.387106	-0.000991
N7	-4.007919	-1.103169	-0.001772
C8	-2.674870	-1.217012	-0.000769
N9	-5.735913	0.403853	-0.002034
H10	-6.367796	-0.379344	-0.002916
H11	-6.115654	1.333655	-0.001029
O12	-1.477661	2.163979	0.002765
H13	0.194048	-2.773321	0.000666
H14	0.487374	-0.246395	0.002129
C15	2.349153	1.594202	0.000032
C16	3.750355	1.867433	-0.002316
C17	4.586209	0.803707	-0.003214
H18	4.134597	2.876818	-0.003585
H19	5.662606	0.923355	-0.005096
N20	1.904952	0.338397	0.001464
C21	2.755410	-0.731285	0.001218
O22	2.347758	-1.883890	0.003507
N23	4.128808	-0.472099	-0.002013
C24	5.031579	-1.621946	-0.000263
H25	4.865136	-2.222179	0.893854
H26	4.843817	-2.240795	-0.877120
H27	6.058493	-1.260542	-0.016669
N28	1.455324	2.585406	0.000769
H29	1.762403	3.542264	-0.000164
H30	0.454666	2.400716	0.002211
N31	-3.561985	1.223114	0.000434
H32	-3.933047	2.164386	0.000857
H33	-2.338228	-3.318357	-0.001991

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

C1	-0.254825	1.467141	0.000049
C2	0.783781	0.471729	0.000022
C3	-1.716851	-0.544240	0.000060
C4	2.682189	-0.635321	-0.000102
N5	2.158740	0.578705	-0.000098
N6	1.685991	-1.531529	0.000026
N7	-0.734678	-1.428092	0.000215
C8	0.472311	-0.865769	0.000106
N9	-2.980226	-0.979495	-0.000368
H10	-3.136298	-1.974278	0.000442
H11	-3.775597	-0.364909	0.000135
O12	-0.143762	2.663637	0.000042
H13	3.734855	-0.867588	-0.000212
H14	2.679649	1.446474	-0.000144
N15	-1.508698	0.814562	0.000058
H16	-2.299171	1.447378	-0.000148
H17	1.799121	-2.536472	-0.000046

TS2_PT7

C1	-1.734214	-0.993244	-0.004620
C2	-1.680945	0.448123	-0.002830
C3	-4.201552	-0.629217	0.000927
C4	-1.197076	2.559157	0.001177
N5	-0.644995	1.372316	-0.002623
N6	-2.546103	2.471284	0.003570
N7	-4.138418	0.679561	0.001396
C8	-2.880811	1.142536	0.001283
N9	-5.401428	-1.236533	0.014047
H10	-6.220662	-0.653363	-0.011016
H11	-5.512681	-2.232279	-0.050414
O12	-0.860800	-1.831620	-0.006279
H13	-0.653020	3.490495	0.002304
H14	0.610234	1.360372	-0.004268
C15	2.633485	-1.726115	0.001704
C16	4.062414	-1.672718	0.004273
C17	4.624667	-0.442835	0.003450
H18	4.675556	-2.562560	0.006686
H19	5.697111	-0.296272	0.005219
N20	1.908871	-0.612297	-0.001171
C21	2.497574	0.568179	-0.001808
O22	1.808870	1.632934	-0.004424
N23	3.869172	0.691488	0.000408
C24	4.470287	2.025915	-0.000598
H25	4.157681	2.572528	-0.889671
H26	4.153614	2.575664	0.885086
H27	5.553519	1.918800	0.002116
N28	1.954726	-2.872475	0.001975
H29	2.414202	-3.765522	0.003988
H30	0.942432	-2.807332	-0.000419
N31	-3.084966	-1.421634	-0.002712
H32	-3.180359	-2.428199	0.007098
H33	-3.203177	3.236517	0.006939

HG-9HG·[1MC+$H_{O2'}$]$^+$

C1	1.741666	-0.958324	0.012545
C2	1.711154	0.479713	0.009361
C3	4.212665	-0.647717	-0.005232
C4	1.257524	2.576870	0.000903
N5	0.677933	1.406725	0.011098
N6	2.614929	2.478989	-0.007646
N7	4.177993	0.659197	-0.004741
C8	2.927340	1.149748	-0.002964
N9	5.401464	-1.286406	-0.046026
H10	6.226052	-0.714828	0.032240
H11	5.487262	-2.266794	0.155864
O12	0.851251	-1.786578	0.017257
H13	0.742839	3.525626	-0.000854
H14	-0.899460	1.472373	0.014924
C15	-2.598742	-1.722811	-0.001885
C16	-4.028895	-1.721029	-0.011387
C17	-4.639921	-0.514598	-0.012246
H18	-4.607884	-2.633575	-0.017859
H19	-5.716886	-0.409139	-0.019443
N20	-1.922933	-0.571558	0.006007
C21	-2.565935	0.562992	0.004880
O22	-1.917311	1.680269	0.012641
N23	-3.929341	0.651542	-0.004504
C24	-4.582763	1.964289	-0.003988
H25	-4.306890	2.514616	0.894763
H26	-4.274948	2.530541	-0.882091
H27	-5.660156	1.813063	-0.025166
N28	-1.866684	-2.828513	-0.000188
H29	-2.281979	-3.743544	-0.006100
H30	-0.854981	-2.708704	0.006577
N31	3.079954	-1.417660	0.004755
H32	3.156038	-2.425167	-0.026092
H33	3.281692	3.234996	-0.017161

Loose TS for dissociation of
HG-9MG·[1MC + $H_{N3'}$]$^+$ → 9MG + [1MC + $H_{N3'}$]$^+$

Vibrational frequencies (cm^{-1}) of products (51 vibrations of 9MG + 45 vibrations of [1MC + $H_{N3'}$]$^+$):

97.6,111.8,136.2,165.8,205.1,233.5,314.8,
323.7,347.7,367.6,465.7,499.2,519.5,571.2,
592.6,626.7,654.5,677.4,704.6,710.9,749.5,
790,825.6,991.8,1021.5,1032.8,1064.4,1103.8,
1109.7,1198.6,1254.2,1281.7,1318.8,1350.5,1392.1,
1416.1,1419.1,1447.3,1471.5,1519.5,1547.3,1558.1,
1605.1,1746.5,2915.6,2988.5,3010.4,3089.1,3440.3,
3457.2,3546.7,57.6,109.1,154,256,308.9,
344.9,394.1,423.6,446.9,470.2,528.9,595.4,
638.2,673,734.8,737.7,758.1,765.1,947.8,
956.4,1025.3,1042.7,1101.4,1110.3,1159.3,1194.2,
1307.6,1333,1380,1399.5,1410.3,1444.1,1518.2,
1552.7,1605.3,1638.8,1798.2,2937.6,3024.1,3038.5,
3076.1,3096.9,3427.1,3437.2,3547.4

Five translational modes (cm^{-1}):

10.1, 14.2, 32.6, 34.3, 42.9

Moments of inetria (amu·Å^2):

815.3, 3323.3, 4131.7

Loose TS for dissociation of
HG-[9MG + H_{N7}]$^+$·1MC → [9MG + H_{N7}]$^+$ + 1MC

Vibrational frequencies (cm^{-1}) of Products (54 vibrations of [9MG + H_{N7}]$^+$ + 42 vibrations of 1MC):

87.5,101.1,131.7,170.5,202.3,235.7,248.1,
314.6,344.5,363.9,461,465.8,505.9,569.9,
597.1,607,645.2,649.1,681.1,688.9,709.1,
739.5,815.7,834.9,976.4,1027.1,1046.6,1050.5,
1103.9,1105.7,1130.9,1236,1269.7,1315.7,1346.4,
1375,1400,1412.5,1437.7,1451.7,1515.7,1531.7,
1560.4,1606.4,1614.9,1767.3,2938.1,3026.4,3038.3,
3129.8,3435.8,3459.4,3465.9,3579.5,91.6,125.8,
177,188.8,242.8,323.1,355.5,394,461.6,
501.6,546.7,590.6,687.9,732.9,738.5,753.2,
764.3,920.3,921.9,1021.9,1041.1,1100.1,1117,
1185.3,1219.1,1291.3,1346.2,1398.8,1401.5,1444.7,
1465.2,1512.2,1564.4,1638.3,1707.1,2919.1,2996.4,
3006.7,3056.5,3082.3,3461.5,3590.9

Five translational modes (cm^{-1}):

9.4, 13.4, 34.9, 40.2, 44.5

Moments of inertia (amu·Å^2):

823.6, 3245.4, 4062.5

Loose TS for dissociation of
HG-9MG·[1MC + $H_{O2'}$]$^+$ → 9MG + [1MC + $H_{O2'}$]$^+$

Vibrational frequencies (cm^{-1}) of Products (51 vibrations of 9MG + 45 vibrations of [1MC + $H_{O2'}$]$^+$):

97.6,111.8,136.2,165.8,205.1,233.5,314.8,
323.7,347.7,367.6,465.7,499.2,519.5,571.2,
592.6,626.7,654.5,677.4,704.6,710.9,749.5,
790,825.6,991.8,1021.5,1032.8,1064.4,1103.8,
1109.7,1198.6,1254.2,1281.7,1318.8,1350.5,1392.1,
1416.1,1419.1,1447.3,1471.5,1519.5,1547.3,1558.1,
1605.1,1746.5,2915.6,2988.5,3010.4,3089.1,3440.3,
3457.2,3546.7,28.6,103,212.4,252.6,314.5,
339,416.3,462.1,469.7,518.3,535.5,566.8,
587.8,687.8,744.3,747.9,763.4,791.5,939,
942.8,1020,1049.7,1101.1,1131.9,1176.7,1204.9,
1287.9,1318.5,1385.2,1405.8,1426.3,1436.9,1486,
1508.2,1551.6,1614.1,1657.9,2939.6,3027.1,3041.1,
3083.3,3096.5,3438.7,3560.6,3639.7

Five translational modes (cm^{-1}):

7.3, 9.5, 28.0, 40.6, 49.8

Moments of inertia (amu·Å^2):

866.8, 3133.7, 3993.2