Supporting Information

Reactions of Water with Radical Cations of Guanine, 9-Methylguanine, 2′-Deoxyguanosine and Guanosine: Keto-Enol Isomerization, C8-Hydroxylation, and Effects of N9-Substitution

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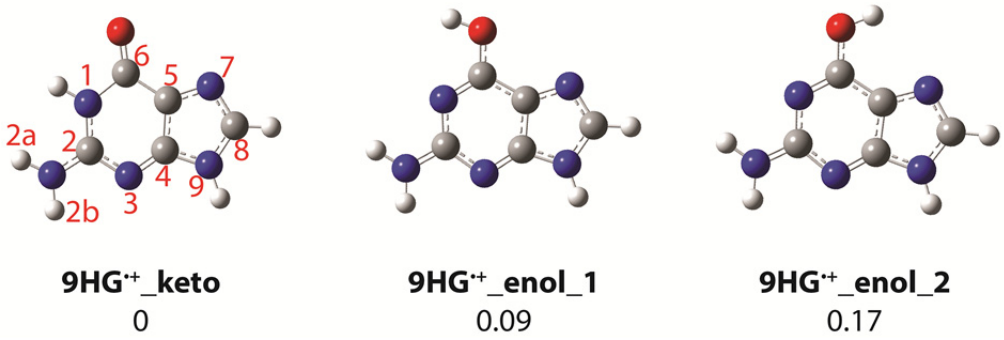

Fig. S1 Low-lying tautomers and rotamers of $9HG^{\bullet+}$. Atomic numbering scheme and nomenclature are presented. Each conformer has a number suffix to denote the order of stability within its structure category. Relative energies (eV, with respect to global minima) were evaluated at ωB97XD/6-31+G(d,p) with 298 K thermal corrections.

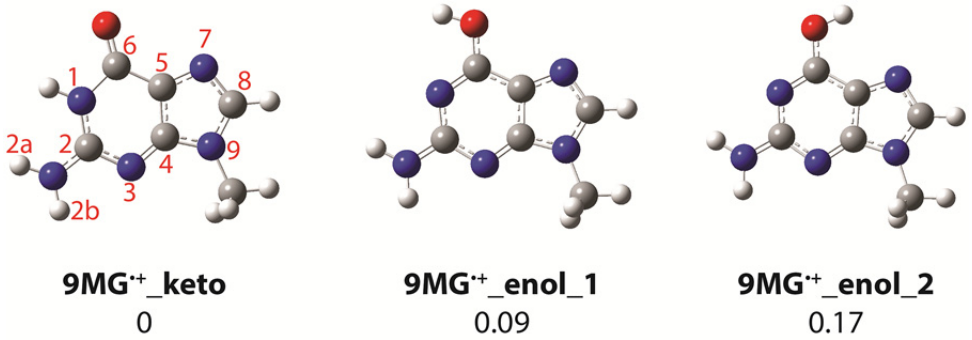

Fig. S2 Low-lying tautomers and rotamers of $9MG^{\bullet+}$. Atomic numbering scheme and nomenclature are presented. Each conformer has a number suffix to denote the order of stability within its structure category. Relative energies (eV, with respect to global minima) were evaluated at ωB97XD/6-31+G(d,p) with 298 K thermal corrections.

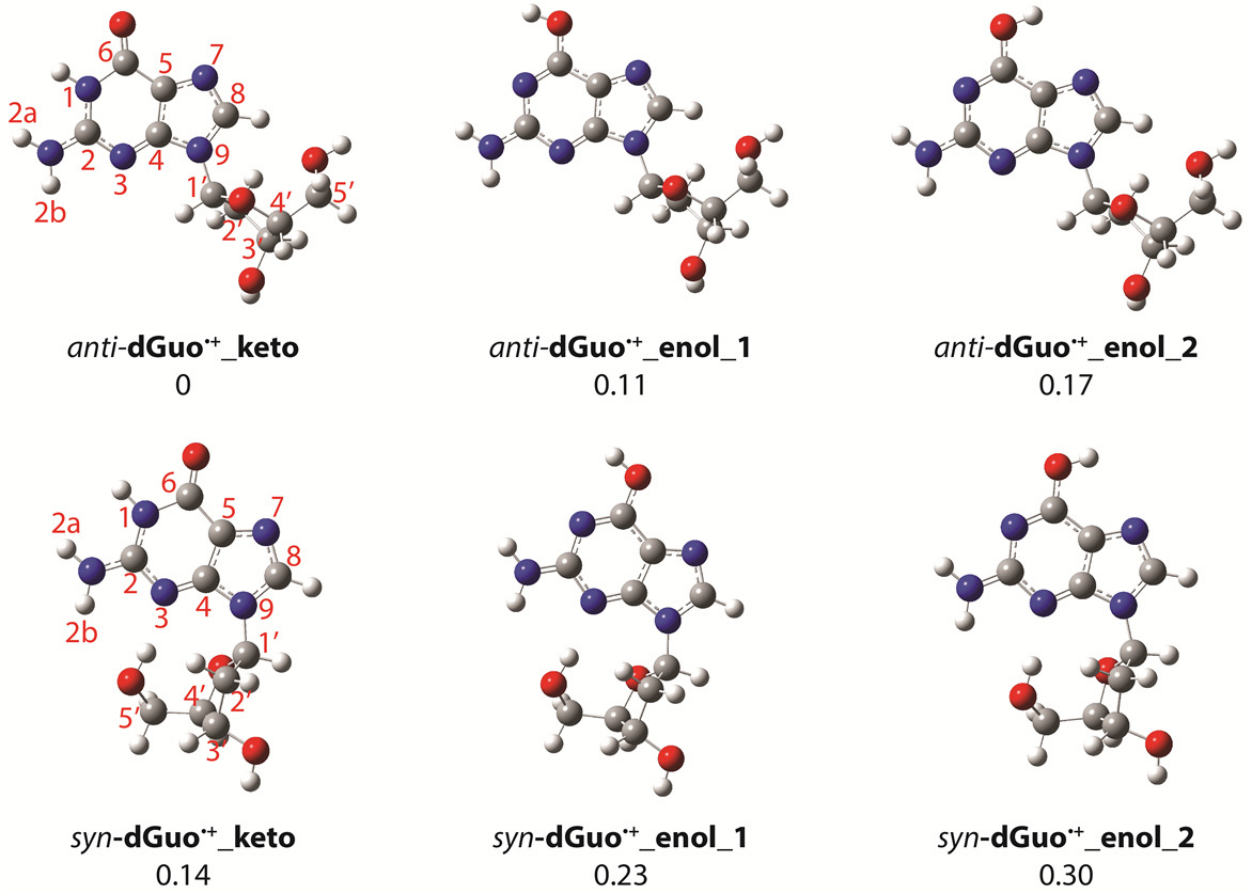

Fig. S3 Low-lying tautomers and rotamers of $dGuo^{\bullet+}$. Atomic numbering scheme and nomenclature are presented. Each conformer has a number suffix to denote the order of stability within its structure category. Relative energies (eV, with respect to global minima) were evaluated at ωB97XD/6-31+G(d,p) with 298 K thermal corrections.

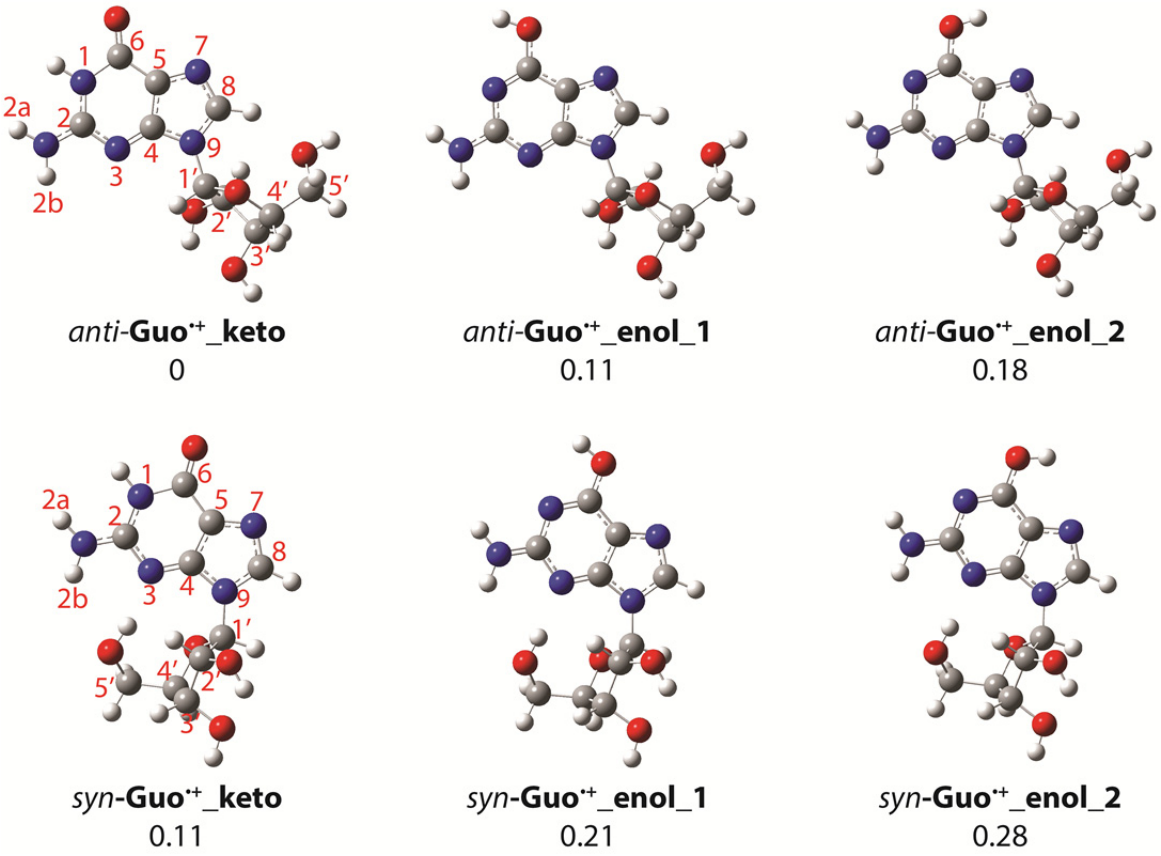

Fig. S4 Low-lying tautomers and rotamers of $Guo^{\bullet+}$. Atomic numbering scheme and nomenclature are presented. Each conformer has a number suffix to denote the order of stability within its structure category. Relative energies (eV, with respect to global minima) were evaluated at ωB97XD/6-31+G(d,p) with 298 K thermal corrections.

Cartesian coordinates for the structures in Fig. S1, optimized at ωB97XD/6-31+G(d,p).

9HG$^{\bullet+}$_keto

C1	-0.246525	1.479497	0.000004
C2	0.854816	0.518755	0.000002
H3	-2.305573	1.419067	0.000005
C4	-1.679426	-0.548633	0.000006
C5	2.692392	-0.514115	-0.000013
N6	-1.503772	0.796299	0.000005
N7	2.171493	0.715558	-0.000015
N8	1.751847	-1.500377	0.000006
N9	-0.652665	-1.437674	0.000017
C10	0.531203	-0.880468	0.000012
N11	-2.901167	-1.058213	-0.000036
H12	-2.995044	-2.065277	0.000073
H13	-3.739392	-0.495433	-0.000028
O14	-0.200466	2.678487	0.000007
H15	3.753107	-0.726499	-0.000026
H16	1.915718	-2.499117	0.000006

9HG$^{\bullet+}$_enol_1

C1	-0.372887	1.332424	-0.000003
C2	0.800774	0.493895	-0.000003
C3	-1.656236	-0.574521	0.000006
C4	2.680229	-0.458597	-0.000006
N5	-1.560826	0.781169	0.000002
N6	2.109729	0.751019	-0.000007
N7	1.788705	-1.483340	-0.000001
N8	-0.630503	-1.490286	0.000006
C9	0.536193	-0.915212	0.000001
N10	-2.874420	-1.085256	0.000011
H11	-3.000036	-2.088901	0.000013
H12	-3.678960	-0.472296	0.000012
O13	-0.218106	2.625883	-0.000007
H14	3.749442	-0.623487	-0.000008
H15	1.998901	-2.473098	0.000001
H16	-1.081726	3.069639	-0.000006

9HG$^{\bullet+}$_enol_2

C1	-0.342277	1.345176	-0.000003
C2	0.791115	0.453372	-0.000003
C3	-1.685989	-0.511239	0.000005
C4	2.648428	-0.543400	-0.000005
N5	-1.545944	0.838292	0.000002
N6	2.107499	0.679751	-0.000007
N7	1.729204	-1.542183	0.000000
N8	-0.697295	-1.474502	0.000005
C9	0.488958	-0.942356	0.000001
N10	-2.922661	-0.974183	0.000010
H11	-3.091655	-1.971622	0.000012
H12	-3.698690	-0.324001	0.000010
O13	-0.207389	2.644654	-0.000006
H14	3.712780	-0.736656	-0.000007
H15	1.915294	-2.536990	0.000002
H16	0.724357	2.912487	-0.000009

Cartesian coordinates for the structures in Fig. S2, optimized at ωB97XD/6-31+G(d,p).

9MG$^{\bullet+}$_keto

C1	-1.205070	1.373596	0.001909
C2	0.216428	1.034962	-0.000522
H3	-2.998666	0.360694	0.003252
C4	-1.529625	-1.090377	-0.000782
C5	2.319045	0.954060	-0.004547
N6	-1.999354	0.182769	0.001621
N7	1.291141	1.814595	-0.002535
N8	1.951099	-0.354609	-0.005088
N9	-0.209725	-1.400171	-0.001351
C10	0.580661	-0.354448	-0.001494
N11	-2.379566	-2.107281	-0.002544
H12	-1.998213	-3.043648	-0.003980
H13	-3.382593	-1.994381	-0.003027
O14	-1.725507	2.455145	0.004289
H15	3.359046	1.254418	-0.006786
C16	2.813108	-1.534800	0.008352
H17	2.706734	-2.055129	0.960908
H18	2.530419	-2.196847	-0.810291
H19	3.844872	-1.211340	-0.122617

9MG$^{\bullet+}$_enol_1

C1	1.290091	-1.138892	0.001683
C2	-0.142735	-0.985426	-0.000358
C3	1.472004	1.153543	-0.000681
C4	-2.245828	-1.057256	-0.004806
N5	2.054303	-0.074437	0.001540
N6	-1.157711	-1.845334	-0.002895
N7	-1.978449	0.269523	-0.004670
N8	0.129785	1.447107	-0.000954
C9	-0.604133	0.371507	-0.000922
N10	2.285987	2.195561	-0.002744
H11	1.905537	3.132216	-0.004428
H12	3.287090	2.053533	-0.002964
O13	1.794559	-2.340862	0.004066
H14	-3.259871	-1.436349	-0.007487
C15	-2.923021	1.384184	0.008051
H16	-2.851209	1.913572	0.958917
H17	-2.688950	2.062881	-0.812386
H18	-3.929059	0.986750	-0.119552
H19	2.764317	-2.298605	0.005628

9MG$^{\bullet+}$_enol_2

C1	-1.286131	1.151105	0.001647
C2	0.141953	0.958193	-0.000279
C3	-1.503742	-1.130845	-0.000555
C4	2.245819	1.019447	-0.004804
N5	-2.067129	0.103610	0.001578
N6	1.162422	1.814103	-0.002778
N7	1.966003	-0.304143	-0.004727
N8	-0.163915	-1.459007	-0.000960
C9	0.588945	-0.397455	-0.000930
N10	-2.337763	-2.156106	-0.002427
H11	-1.979653	-3.101716	-0.004042
H12	-3.335572	-1.987151	-0.002491
O13	-1.829975	2.339978	0.003902
H14	3.262971	1.389735	-0.007502
C15	2.902410	-1.426380	0.007897
H16	2.825324	-1.955190	0.958632
H17	2.662493	-2.102625	-0.812850
H18	3.911795	-1.037446	-0.119312
H19	-1.160413	3.040990	0.003691

Cartesian coordinates for the structures in Fig. S3, optimized at ωB97XD/6-31+G(d,p).

anti-**dGuo$^{\bullet+}$_keto**

O1	3.140448	-1.988426	0.263691
C2	3.792203	-1.268264	-0.779029
H3	3.565923	-1.712828	-1.754991
H4	4.879527	-1.272390	-0.633525
C5	3.313546	0.171276	-0.771517
H6	3.861401	0.727109	-1.537403
O7	1.916106	0.228549	-1.108670
C8	1.157033	0.709596	-0.039624
H9	0.741628	1.696114	-0.266117
N10	-0.008668	-0.182237	0.102732
C11	0.036825	-1.540927	0.198333
H12	0.991096	-2.058686	0.233253
N13	-1.172865	-2.121615	0.220904
C14	-2.024340	-1.107168	0.119355
C15	-3.483676	-1.094136	0.081465
O16	-4.251920	-2.015476	0.150819
N17	-3.966405	0.243899	-0.063457
H18	-4.978053	0.310048	-0.103108
C19	-3.200679	1.362457	-0.148610
N20	-3.783266	2.546383	-0.292686
H21	-4.782583	2.670308	-0.353659
H22	-3.188400	3.360622	-0.358663
N23	-1.850649	1.350316	-0.092301
C24	-1.331123	0.151151	0.030131
C25	3.446887	0.899850	0.572656
H26	4.235349	0.458602	1.191450
C27	2.061183	0.714596	1.195547
H28	2.013497	-0.249782	1.707256
H29	1.802167	1.509435	1.897171
O30	3.716715	2.255894	0.276660
H31	3.557908	-2.848164	0.366957
H32	3.995565	2.717480	1.072780

anti-**dGuo$^{\bullet+}$_enol_1**

O1	3.109991	-2.009524	0.283760
C2	3.785224	-1.309067	-0.757858
H3	3.560363	-1.757450	-1.732414
H4	4.870773	-1.332264	-0.601555
C5	3.331925	0.138706	-0.766623
H6	3.893632	0.677718	-1.534543
O7	1.937954	0.215915	-1.112172
C8	1.180469	0.716976	-0.050703
H9	0.781746	1.708087	-0.287380
N10	-0.000666	-0.153243	0.093239
C11	0.014068	-1.505903	0.187692
H12	0.956279	-2.045633	0.223073
N13	-1.208604	-2.067395	0.211513
C14	-2.038436	-1.032098	0.110650
C15	-3.472005	-0.910965	0.066933
O16	-4.200496	-1.991038	0.152938
N17	-4.020896	0.271975	-0.060874
C18	-3.213423	1.362997	-0.145048
N19	-3.814897	2.533473	-0.288488
H20	-4.823293	2.579732	-0.333911
H21	-3.262419	3.376461	-0.360700
N22	-1.844351	1.399171	-0.097157
C23	-1.323933	0.210533	0.022141
C24	3.470066	0.877718	0.571238
H25	4.249191	0.430827	1.197996
C26	2.078973	0.717941	1.188749
H27	2.014689	-0.242590	1.705978
H28	1.827835	1.521131	1.883751
O29	3.761819	2.226334	0.263178
H30	3.515795	-2.872794	0.402350
H31	4.031536	2.694862	1.058399
H32	-5.141938	-1.760486	0.106678

anti-**dGuo$^{\bullet+}$_enol_2**

O1	3.094244	-2.009323	0.301565
C2	3.784321	-1.316470	-0.736062
H3	3.570189	-1.770761	-1.710286
H4	4.867720	-1.341790	-0.566590
C5	3.335062	0.132290	-0.759760
H6	3.902898	0.663345	-1.528698
O7	1.943283	0.208974	-1.115370
C8	1.180591	0.724402	-0.065034
H9	0.786819	1.714404	-0.314573
N10	-0.005515	-0.140612	0.078534
C11	0.005957	-1.492661	0.172274
H12	0.946693	-2.035402	0.206457
N13	-1.220372	-2.046463	0.198873
C14	-2.043469	-1.003555	0.102159
C15	-3.478852	-0.906017	0.065732
O16	-4.249042	-1.961769	0.145919
N17	-4.035508	0.269707	-0.054450
C18	-3.232443	1.361771	-0.138237
N19	-3.843484	2.527396	-0.273670
H20	-4.853604	2.559043	-0.311954
H21	-3.301364	3.377263	-0.346068
N22	-1.857913	1.416498	-0.099178
C23	-1.329039	0.231896	0.014031
C24	3.465684	0.883725	0.571980
H25	4.238886	0.440828	1.208887
C26	2.069727	0.733763	1.181003
H27	1.998488	-0.222296	1.705532
H28	1.816078	1.543613	1.867280
O29	3.763148	2.228120	0.252709
H30	3.506162	-2.866665	0.440313
H31	4.029338	2.704255	1.044621
H32	-3.727054	-2.774410	0.227207

syn-**dGuo$^{\bullet+}$_keto**

C1	-3.509340	-0.295440	0.004018
C2	-2.285499	-1.092896	0.082435
H3	-4.015466	1.690568	-0.220223
C4	-1.952093	1.623966	-0.235810
C5	-0.786525	-2.558309	0.260214

N6	-3.197275	1.092390	-0.164921
N7	-2.116940	-2.399944	0.247708
N8	-0.083068	-1.405311	0.094027
N9	-0.826918	0.872120	-0.167494
C10	-1.024905	-0.413863	-0.014699
N11	-1.778854	2.928902	-0.377437
H12	-0.829365	3.285184	-0.414006
H13	-2.542839	3.586386	-0.433884
O14	-4.650885	-0.660612	0.061809
H15	-0.292601	-3.512727	0.390545
C16	1.382736	-1.264755	0.093042
O17	1.717621	-0.365045	1.109367
C18	1.967949	-0.692414	-1.195582
H19	1.770761	-2.269736	0.299058
C20	2.921657	0.355238	0.750938
C21	3.283450	-0.121387	-0.675825
H22	1.335338	0.108753	-1.584127
H23	3.708837	0.056597	1.451810
H24	3.644935	0.704569	-1.296909
O25	4.199303	-1.198247	-0.650150
H26	5.087260	-0.881712	-0.459379
C27	2.650515	1.845466	0.900085
H28	2.378521	2.052798	1.943163
H29	3.563386	2.402980	0.672494
O30	1.648039	2.295956	0.010687
H31	0.881106	1.716998	0.126546
H32	2.131231	-1.447814	-1.964865

***syn*-dGuo$^{\bullet+}$_enol_1**

C1	-3.419101	-0.177271	-0.007355
C2	-2.266220	-1.039765	0.077126
C3	-1.996409	1.612321	-0.231672
C4	-0.784516	-2.522376	0.251476
N5	-3.257397	1.114362	-0.160268
N6	-2.116213	-2.351875	0.238904
N7	-0.067883	-1.383812	0.090122
N8	-0.820397	0.907511	-0.164731
C9	-1.000640	-0.373903	-0.017182
N10	-1.866983	2.919182	-0.379477
H11	-0.944715	3.336073	-0.433483
H12	-2.690625	3.503320	-0.433114
O13	-4.605817	-0.710326	0.071033
H14	-0.303655	-3.483835	0.379654
C15	1.398876	-1.261116	0.091983
O16	1.740466	-0.371931	1.113896
C17	1.990366	-0.687572	-1.193188
H18	1.775109	-2.271879	0.292258
C19	2.942373	0.351911	0.755780
C20	3.308198	-0.127705	-0.667983
H21	1.364617	0.120269	-1.579023
H22	3.727580	0.057812	1.460868
H23	3.679056	0.695252	-1.287352
O24	4.215091	-1.212638	-0.638311
H25	5.103425	-0.903352	-0.437777
C26	2.669975	1.842528	0.895448
H27	2.369179	2.050628	1.930611
H28	3.592777	2.394799	0.696276
O29	1.701245	2.302137	-0.023966
H30	0.902880	1.767978	0.095770
H31	2.149658	-1.441134	-1.965147
H32	-5.288478	-0.023744	0.000795

***syn*-dGuo$^{\bullet+}$_enol_2**

C1	-3.427174	-0.150251	-0.008397
C2	-2.265447	-1.000724	0.072653
C3	-2.006198	1.631160	-0.231086
C4	-0.803118	-2.502975	0.245793
N5	-3.266814	1.137904	-0.159992
N6	-2.132735	-2.316500	0.231764
N7	-0.077120	-1.370777	0.088230
N8	-0.819775	0.933161	-0.163448
C9	-0.999137	-0.348064	-0.018279
N10	-1.880678	2.937736	-0.380992
H11	-0.961484	3.360726	-0.438132
H12	-2.710765	3.514094	-0.435670
O13	-4.641937	-0.627036	0.064110
H14	-0.331294	-3.469010	0.371969
C15	1.391756	-1.263064	0.090626
O16	1.740150	-0.380099	1.114565
C17	1.987178	-0.691145	-1.193248
H18	1.757789	-2.278214	0.287983
C19	2.947911	0.335867	0.757565
C20	3.310265	-0.145414	-0.666319
H21	1.369126	0.124523	-1.575158
H22	3.730049	0.034981	1.463100
H23	3.689752	0.674513	-1.284358
O24	4.205621	-1.239904	-0.637259
H25	5.097610	-0.940064	-0.438581
C26	2.686742	1.828343	0.897430
H27	2.382743	2.038199	1.931280
H28	3.615351	2.372701	0.703630
O29	1.727714	2.297424	-0.026891
H30	0.916684	1.784819	0.099676
H31	2.138984	-1.443415	-1.967971
H32	-4.643747	-1.590000	0.176661

Cartesian coordinates for the structures in Fig. S4, optimized at ωB97XD/6-31+G(d,p).

anti-**Guo$^{\bullet+}$_keto**

O1	3.035367	-2.087249	0.455746
C2	3.771234	-1.527828	-0.625177
H3	3.625974	-2.114054	-1.540080
H4	4.844101	-1.493551	-0.396376
C5	3.280964	-0.112421	-0.870549
H6	3.862178	0.319883	-1.691202
O7	1.902681	-0.147250	-1.290259
C8	1.083186	0.503531	-0.370392
H9	0.707929	1.459488	-0.751534
N10	-0.099329	-0.336755	-0.150275
C11	-0.093406	-1.675056	0.102790
H12	0.842703	-2.221480	0.155946
N13	-1.317723	-2.197586	0.271120
C14	-2.138089	-1.163295	0.122412
C15	-3.594007	-1.089201	0.198700
O16	-4.386935	-1.964838	0.419441
N17	-4.037573	0.249447	-0.034484
H18	-5.045156	0.358632	0.011727
C19	-3.241839	1.317879	-0.299125
N20	-3.789975	2.508997	-0.504901
H21	-4.784420	2.675994	-0.476892
H22	-3.171514	3.286358	-0.690657
N23	-1.894354	1.247793	-0.366988
C24	-1.410575	0.047497	-0.153053
C25	3.325483	0.818746	0.351503
H26	4.083438	0.516342	1.080141
C27	1.906940	0.703549	0.921930
H28	1.841415	-0.200383	1.533251
O29	3.471896	2.176602	-0.022246
H30	3.439289	-2.916119	0.728029
H31	4.399013	2.422626	-0.076735
O32	1.483740	1.784078	1.685992
H33	1.934363	2.571840	1.349442

anti-**Guo$^{\bullet+}$_enol_1**

O1	3.004472	-2.113448	0.461795
C2	3.757141	-1.567178	-0.614457
H3	3.607958	-2.151852	-1.529752
H4	4.828905	-1.551524	-0.378421
C5	3.293195	-0.143827	-0.865457
H6	3.885746	0.275259	-1.684917
O7	1.916555	-0.156013	-1.290522
C8	1.103990	0.510840	-0.375437
H9	0.745563	1.471581	-0.760991
N10	-0.093466	-0.307350	-0.156796
C11	-0.118096	-1.638396	0.098015
H12	0.805087	-2.206386	0.153520
N13	-1.354549	-2.140869	0.266170
C14	-2.152547	-1.086861	0.112294
C15	-3.579552	-0.908391	0.165103
O16	-4.336953	-1.941734	0.417791
N17	-4.094409	0.279096	-0.038574
C18	-3.257423	1.319058	-0.298455
N19	-3.824885	2.497897	-0.499814
H20	-4.830265	2.587817	-0.454350
H21	-3.248424	3.305397	-0.691408
N22	-1.889619	1.296739	-0.375949
C23	-1.404325	0.106988	-0.163775
C24	3.349318	0.790704	0.353446
H25	4.099742	0.478498	1.085821
C26	1.927165	0.701209	0.919231
H27	1.843887	-0.199869	1.532401
O28	3.519582	2.144362	-0.024889
H29	3.395286	-2.946745	0.739407
H30	4.450733	2.375016	-0.076984
O31	1.520428	1.789694	1.680273
H32	1.978164	2.571081	1.338638
H33	-5.269756	-1.674634	0.423141

anti-**Guo$^{\bullet+}$_enol_2**

O1	2.987810	-2.116500	0.464928
C2	3.750914	-1.572196	-0.605553
H3	3.607692	-2.157481	-1.521364
H4	4.820648	-1.559475	-0.360748
C5	3.292926	-0.147836	-0.861483
H6	3.889298	0.266991	-1.680294
O7	1.917272	-0.157413	-1.290854
C8	1.104768	0.516845	-0.381697
H9	0.751673	1.477733	-0.771886
N10	-0.097963	-0.295384	-0.164781
C11	-0.127054	-1.626160	0.087719
H12	0.793818	-2.198211	0.141568
N13	-1.367080	-2.119942	0.256175
C14	-2.156987	-1.057682	0.104503
C15	-3.586177	-0.901642	0.164091
O16	-4.385045	-1.909554	0.410672
N17	-4.107992	0.279469	-0.033461
C18	-3.274452	1.320436	-0.291062
N19	-3.850134	2.495605	-0.485644
H20	-4.857251	2.571899	-0.435128
H21	-3.282935	3.309967	-0.676696
N22	-1.901096	1.315505	-0.375525
C23	-1.408150	0.128740	-0.168882
C24	3.347922	0.790446	0.354730
H25	4.094904	0.478134	1.090596
C26	1.923537	0.707322	0.915853
H27	1.834843	-0.192608	1.530039
O28	3.523134	2.142093	-0.027261
H29	3.383066	-2.943385	0.755082
H30	4.454947	2.370679	-0.077273
O31	1.517469	1.797895	1.673489
H32	1.977417	2.578072	1.331975
H33	-3.886877	-2.730893	0.539675

syn-**Guo$^{\bullet+}$_keto**

C1	3.610210	-0.387724	0.034109
C2	2.354674	-1.096453	-0.211365

H3	4.204381	1.534344	0.484411
C4	2.147298	1.597717	0.325189
C5	0.794906	-2.452024	-0.608168
N6	3.362644	0.997874	0.300218
N7	2.126687	-2.376345	-0.481000
N8	0.148819	-1.267653	-0.430411
N9	0.992265	0.932015	0.083307
C10	1.131208	-0.347502	-0.164813
N11	2.037475	2.890442	0.591589
H12	1.110178	3.301256	0.605581
H13	2.829741	3.483796	0.789770
O14	4.730292	-0.818090	0.036591
H15	0.258410	-3.365577	-0.829097
C16	-1.301155	-1.052494	-0.453868
O17	-1.577146	0.000223	-1.321272
C18	-1.881408	-0.649410	0.914953
H19	-1.737951	-2.003193	-0.787330
C20	-2.774666	0.695341	-0.881929
C21	-3.166079	0.063612	0.469170
H22	-1.216070	0.075996	1.392031
H23	-3.562655	0.506263	-1.618347
H24	-3.486842	0.814024	1.196949
O25	-2.054848	-1.725078	1.774321
H26	-2.938417	-2.087966	1.613763
O27	-4.128908	-0.964418	0.319664
H28	-5.021776	-0.617126	0.393270
C29	-2.451027	2.181595	-0.836904
H30	-2.168043	2.511723	-1.844606
H31	-3.340857	2.740817	-0.534999
O32	-1.432938	2.465258	0.101102
H33	-0.680710	1.892195	-0.108810

***syn*-Guo$^{\bullet+}$_enol_1**

C1	3.526668	-0.262125	0.050233
C2	2.339596	-1.039996	-0.204607
C3	2.191414	1.588057	0.317207
C4	0.796823	-2.414092	-0.601838
N5	3.423923	1.019915	0.303435
N6	2.130217	-2.326500	-0.469101
N7	0.136991	-1.242577	-0.435173
N8	0.989004	0.970476	0.077638
C9	1.110759	-0.303360	-0.166657
N10	2.123154	2.879925	0.588902
H11	1.224717	3.347307	0.619640
H12	2.970244	3.398627	0.778050
O13	4.684399	-0.859837	0.023941
H14	0.273498	-3.335931	-0.820219
C15	-1.314677	-1.045531	-0.462939
O16	-1.598542	0.007655	-1.325262
C17	-1.901822	-0.657605	0.907423
H18	-1.739417	-1.999821	-0.802269
C19	-2.795297	0.698787	-0.878433
C20	-3.189332	0.050619	0.463390
H21	-1.242989	0.067931	1.393022
H22	-3.581338	0.520430	-1.619705
H23	-3.517893	0.791843	1.197012
O24	-2.071142	-1.743056	1.755932
H25	-2.952819	-2.108043	1.589869
O26	-4.144741	-0.982778	0.299987
H27	-5.039916	-0.640705	0.369438
C28	-2.472845	2.183964	-0.808847
H29	-2.164268	2.524607	-1.805659
H30	-3.372521	2.738007	-0.526569
O31	-1.485183	2.463362	0.160461
H32	-0.700776	1.937430	-0.055761
H33	5.394401	-0.225432	0.213179

***syn*-Guo$^{\bullet+}$_enol_2**

C1	3.535040	-0.239415	0.058547
C2	2.338789	-1.002696	-0.196437
C3	2.204821	1.606934	0.311578
C4	0.812246	-2.394900	-0.594706
N5	3.435869	1.040403	0.304777
N6	2.144106	-2.294106	-0.455170
N7	0.145149	-1.227105	-0.437600
N8	0.991797	0.998423	0.070918
C9	1.110261	-0.276028	-0.168430
N10	2.142502	2.899365	0.579795
H11	1.248264	3.374653	0.609301
H12	2.996229	3.408748	0.769049
O13	4.721657	-0.787193	0.054014
H14	0.296233	-3.321310	-0.810376
C15	-1.308995	-1.042849	-0.469709
O16	-1.597820	0.013654	-1.324594
C17	-1.902038	-0.670672	0.902318
H18	-1.724147	-1.998558	-0.817147
C19	-2.800603	0.693591	-0.874939
C20	-3.193456	0.031827	0.460645
H21	-1.250023	0.055822	1.395816
H22	-3.583217	0.515808	-1.619886
H23	-3.528472	0.765294	1.199107
O24	-2.064999	-1.765522	1.740014
H25	-2.945840	-2.131960	1.572274
O26	-4.141148	-1.006929	0.287278
H27	-5.038898	-0.671848	0.358071
C28	-2.488159	2.180018	-0.791213
H29	-2.176593	2.531460	-1.783322
H30	-3.393315	2.725340	-0.509523
O31	-1.508751	2.457997	0.186397
H32	-0.712641	1.953881	-0.038088
H33	4.677507	-1.737113	-0.135106

Cartesian coordinates for the structures in Fig. 2, optimized at ωB97XD/6-31+G(d,p).

9HG$^{\bullet+}$·W12a

C1	0.057752	1.313670	-0.000019
C2	-1.237153	0.631594	-0.000001
H3	2.068657	0.753590	-0.000028
C4	0.980995	-0.979828	-0.000019
C5	-3.264413	0.050824	0.000025
N6	1.118356	0.369389	-0.000026
N7	-2.474995	1.126176	0.000017
N8	-2.576978	-1.126191	0.000012
N9	-0.221931	-1.619087	-0.000012
C10	-1.244915	-0.804097	-0.000003
N11	2.066269	-1.733328	-0.000017
H12	1.952194	-2.737146	-0.000014
H13	2.993554	-1.313124	-0.000012
O14	0.276107	2.496426	-0.000027
H15	-4.345392	0.088486	0.000041
H16	-2.966333	-2.059847	0.000017
O17	3.995365	0.432387	0.000042
H18	4.498500	0.722928	-0.769063
H19	4.498405	0.722925	0.769211

9HG$^{\bullet+}$·W16

C1	-0.429751	-1.044077	-0.000001
C2	0.996756	-0.723291	-0.000001
H3	-2.237034	-0.053917	-0.000014
C4	-0.737314	1.396791	-0.000001
C5	3.104682	-0.679664	0.000000
N6	-1.217011	0.135122	-0.000007
N7	2.066610	-1.518154	0.000000
N8	2.741407	0.633767	0.000000
N9	0.588791	1.709892	0.000000
C10	1.371220	0.662598	-0.000001
N11	-1.581984	2.417484	0.000004
H12	-1.202138	3.354074	0.000008
H13	-2.584000	2.294865	0.000014
O14	-0.945371	-2.134143	0.000003
H15	4.140416	-0.991647	0.000001
H16	3.356929	1.436604	0.000001
O17	-3.720634	-0.940987	0.000014
H18	-4.680018	-0.883441	-0.000121
H19	-3.484362	-1.876415	0.000030

9HG$^{\bullet+}$·W9

C1	1.758152	1.026519	-0.000063
C2	0.299892	1.109502	0.000007
H3	3.186232	-0.456524	-0.000093
C4	1.361106	-1.424294	0.000022
C5	-1.735703	1.642830	0.000105
N6	2.178095	-0.340076	-0.000048
N7	-0.502156	2.169087	0.000027
N8	-1.757837	0.286590	0.000133
N9	0.009883	-1.344890	0.000085
C10	-0.452898	-0.117291	0.000076
N11	1.885966	-2.642418	0.000030
H12	1.251737	-3.429496	0.000082
H13	2.879150	-2.820677	-0.000012
O14	2.567034	1.914336	-0.000126
H15	-2.643807	2.230407	0.000158
H16	-2.608894	-0.305042	0.000203
O17	-4.170820	-1.024991	-0.000174
H18	-4.657496	-1.327543	-0.772887
H19	-4.657579	-1.327536	0.772487

9HG$^{\bullet+}$·W2b

C1	-1.229264	1.477760	-0.000001
C2	-1.587083	0.060757	0.000003
H3	0.492591	2.599253	-0.000003
C4	1.109807	0.627609	-0.000003
C5	-2.509855	-1.834777	0.000002
N6	0.188526	1.631177	-0.000005
N7	-2.782674	-0.529075	0.000006
N8	-1.175364	-2.109259	-0.000005
N9	0.765796	-0.691199	-0.000009
C10	-0.524049	-0.902532	-0.000003
N11	2.395230	0.909935	0.000010
H12	3.097614	0.151613	0.000032
H13	2.731501	1.862380	0.000019
O14	-1.953123	2.436358	-0.000001
H15	-3.259960	-2.613803	0.000004
H16	-0.740631	-3.022526	-0.000010
O17	4.510753	-0.881015	0.000000
H18	4.959908	-1.236879	0.772326
H19	4.960009	-1.236740	-0.772331

9MG$^{\bullet+}$·W12a

C1	0.610261	1.452293	-0.001944
C2	-0.791531	1.031967	0.000496
H3	2.474569	0.514452	-0.002625
C4	1.075676	-0.978664	0.001088
C5	-2.886951	0.829043	0.004646
N6	1.468848	0.319876	-0.001498
N7	-1.912343	1.747426	0.002493
N8	-2.443349	-0.455688	0.005471
N9	-0.225728	-1.373871	0.001615
C10	-1.074036	-0.375744	0.001682
N11	1.999374	-1.924952	0.003088
H12	1.696579	-2.888361	0.004708
H13	2.989292	-1.687822	0.003142
O14	1.056348	2.569552	-0.004402
H15	-3.942924	1.066665	0.006917
O16	4.311613	-0.182968	-0.000489
H17	4.861473	0.002521	-0.769997
H18	4.860897	0.007710	0.768152
C19	-3.233315	-1.683505	-0.009088
H20	-3.100469	-2.194789	-0.963341
H21	-2.909024	-2.331340	0.805606
H22	-4.282315	-1.423591	0.127096

9MG$^{\bullet+}$·W16

C1	-0.949140	-1.055709	0.000495
C2	0.511283	-1.000652	0.001798
H3	-2.542744	0.250200	-0.000806
C4	-0.804193	1.402111	0.002575
C5	2.591438	-1.322374	0.003853
N6	-1.506317	0.248625	0.000906
N7	1.419410	-1.971408	0.003277
N8	2.479804	0.031987	0.004094
N9	0.554898	1.468099	0.001789
C10	1.133006	0.293229	0.001701
N11	-1.452048	2.559238	0.004969
H12	-0.910455	3.412029	0.005780
H13	-2.459593	2.618302	0.006785
O14	-1.658638	-2.031239	-0.001209
H15	3.555250	-1.814805	0.005308
O16	-4.162578	-0.368024	-0.005709
H17	-5.099746	-0.155294	-0.010914
H18	-4.080126	-1.329429	-0.006654
C19	3.549578	1.025973	-0.011896
H20	3.546272	1.554602	-0.965952
H21	3.397419	1.733630	0.803377
H22	4.501395	0.513612	0.122023

9MG$^{\bullet+}$·W2b

C1	-1.077484	-1.854905	0.000279
C2	-1.529550	-0.465404	-0.003325
H3	0.716753	-2.856704	0.007930
C4	1.200394	-0.847930	0.005764
C5	-2.557219	1.371230	-0.009346
N6	0.348215	-1.911443	0.005701
N7	-2.756575	0.047056	-0.009544
N8	-1.249005	1.738146	-0.004629
N9	0.769764	0.442722	0.004753
C10	-0.533324	0.566882	0.000331
N11	2.502808	-1.047747	0.007161
H12	3.153721	-0.246739	0.004053
H13	2.898826	-1.976612	0.007761
O14	-1.732214	-2.862408	-0.000374
H15	-3.354133	2.103444	-0.013751
O16	4.500451	0.890515	-0.011966
H17	4.951361	1.255090	0.755199
H18	4.957105	1.226573	-0.788716
C19	-0.688582	3.085891	0.014637
H20	-0.193428	3.263846	0.970065
H21	0.030560	3.188766	-0.798235
H22	-1.498519	3.801765	-0.119719

9MG$^{\bullet+}$·W8

O1	-4.868918	0.146761	-0.000176
H2	-5.440253	0.261603	-0.766109
H3	-5.440468	0.261495	0.765612
N4	2.555205	0.334221	-0.000044
C5	2.196721	-0.975283	-0.000041
N6	0.911352	-1.397808	0.000004
C7	0.032098	-0.423775	0.000040
C8	0.275333	0.992858	0.000038
C9	1.661705	1.451988	-0.000006
N10	-0.861579	1.676222	0.000076
C11	-1.816480	0.729079	0.000102
N12	-1.331278	-0.540890	0.000081
H13	3.535115	0.597703	-0.000076
N14	3.134647	-1.913853	-0.000083
H15	2.836883	-2.879634	-0.000078
H16	4.123245	-1.712226	-0.000118
O17	2.089995	2.574091	-0.000013
H18	-2.886991	0.914783	0.000129
C19	-2.098428	-1.785711	0.000123
H20	-1.851206	-2.362273	-0.892073
H21	-1.851461	-2.362066	0.892525
H22	-3.157598	-1.526382	-0.000060

dGuo$^{\bullet+}$·W12a

O1	3.753130	1.820432	-0.202440
C2	4.326607	1.032182	0.836458
H3	4.121182	1.476590	1.817171
H4	5.412950	0.948650	0.707171
C5	3.732665	-0.363041	0.794713
H6	4.225344	-0.975854	1.554804
O7	2.332299	-0.313683	1.114258
C8	1.550205	-0.718143	0.028149
H9	1.062248	-1.675586	0.233574
N10	0.457228	0.256858	-0.114240
C11	0.598621	1.609545	-0.200583
H12	1.585713	2.060923	-0.221461
N13	-0.565492	2.273113	-0.232977
C14	-1.489650	1.319914	-0.148717
C15	-2.948449	1.410239	-0.127830
O16	-3.639045	2.394265	-0.198945
N17	-3.525723	0.119392	-0.000673
H18	-4.548158	0.082265	0.033561
C19	-2.843542	-1.051477	0.084199
N20	-3.529538	-2.177343	0.209116
H21	-4.545718	-2.168712	0.247256
H22	-3.015554	-3.043596	0.276576
N23	-1.491039	-1.143612	0.046061
C24	-0.888262	0.016268	-0.059892
C25	3.827550	-1.072837	-0.562737
H26	4.654355	-0.679225	-1.163470
C27	2.467784	-0.771933	-1.195945
H28	2.500936	0.201778	-1.690824
H29	2.157044	-1.532137	-1.914825
O30	3.994338	-2.451018	-0.291584
H31	4.231912	2.650819	-0.273887
H32	4.229736	-2.917970	-1.098517
O33	-6.186478	-0.992795	0.204375
H34	-6.726672	-0.850101	0.989497
H35	-6.798495	-0.998616	-0.539831

dGuo$^{\bullet+}$·W16

O1	3.569803	-2.018810	0.263184
C2	4.228518	-1.308587	-0.781721

H3	3.994947	-1.751786	-1.756636
H4	5.316060	-1.325981	-0.638038
C5	3.767001	0.136665	-0.776068
H6	4.321870	0.684957	-1.542484
O7	2.371046	0.209641	-1.112493
C8	1.617619	0.702109	-0.043201
H9	1.218235	1.694989	-0.270750
N10	0.439685	-0.169771	0.100731
C11	0.460110	-1.528329	0.199320
H12	1.404369	-2.063479	0.233104
N13	-0.758889	-2.086976	0.226742
C14	-1.593701	-1.056899	0.125364
C15	-3.052641	-1.010007	0.092869
O16	-3.831199	-1.930087	0.173289
N17	-3.516152	0.320446	-0.056971
H18	-4.548025	0.391997	-0.099495
C19	-2.732618	1.419100	-0.137518
N20	-3.302172	2.610936	-0.272926
H21	-4.302749	2.733923	-0.312246
H22	-2.703632	3.421825	-0.336664
N23	-1.377756	1.394278	-0.087653
C24	-0.878622	0.187962	0.031952
C25	3.910401	0.864196	0.567593
H26	4.694234	0.413813	1.185849
C27	2.523175	0.695773	1.191024
H28	2.464154	-0.268453	1.701895
H29	2.273702	1.493006	1.893508
O30	4.197624	2.216725	0.270374
H31	3.973632	-2.885283	0.363533
H32	4.469321	2.677956	1.069151
O33	-6.208680	-0.137587	-0.028189
H34	-7.112927	0.064068	-0.283343
H35	-6.140407	-1.094895	0.076161

dGuo$^{\bullet+}$·W2b

O1	3.659378	-1.774859	0.132708
C2	4.157154	-0.892286	-0.868708
H3	3.985736	-1.307155	-1.868760
H4	5.232939	-0.721758	-0.736841
C5	3.443808	0.442213	-0.761941
H6	3.876262	1.130731	-1.493469
O7	2.051732	0.283938	-1.082364
C8	1.242311	0.566341	0.022725
H9	0.672719	1.486748	-0.136764
N10	0.239576	-0.505536	0.118454
C11	0.499756	-1.842713	0.139617
H12	1.522873	-2.206104	0.141165
N13	-0.601381	-2.606697	0.134846
C14	-1.605196	-1.734989	0.092204
C15	-3.048165	-1.951669	0.062127
O16	-3.657625	-2.988531	0.083759
N17	-3.735491	-0.705064	-0.004533
H18	-4.744920	-0.798170	-0.035000
C19	-3.162699	0.531959	-0.036098
N20	-3.927326	1.604441	-0.114615
H21	-4.933093	1.538933	-0.166449
H22	-3.501587	2.542518	-0.149500
N23	-1.820913	0.726567	0.012903
C24	-1.122754	-0.381007	0.068618
C25	3.481763	1.094662	0.626728
H26	4.344495	0.750969	1.207167
C27	2.158295	0.642515	1.246818
H28	2.281113	-0.346472	1.694881
H29	1.785546	1.337613	2.001398
O30	3.520677	2.494151	0.421210
H31	4.209646	-2.562237	0.165718
H32	3.732174	2.939646	1.246637
O33	-3.074101	4.255960	-0.280122
H34	-2.741828	4.687406	-1.072594
H35	-3.069457	4.915916	0.418959

dGuo$^{\bullet+}$·W3′

O1	-2.500962	-2.576505	-0.497653
C2	-3.175868	-2.250612	0.715235
H3	-2.823536	-2.889346	1.533626
H4	-4.259006	-2.384522	0.604595
C5	-2.906307	-0.801224	1.069473
H6	-3.460311	-0.554286	1.979354
O7	-1.505626	-0.619215	1.351858
C8	-0.915110	0.245709	0.428678
H9	-0.628116	1.189151	0.902643
N10	0.351950	-0.381005	0.001096
C11	0.493458	-1.664476	-0.431619
H12	-0.374698	-2.309559	-0.535647
N13	1.766596	-2.012957	-0.682111
C14	2.466663	-0.924232	-0.387283
C15	3.903374	-0.676120	-0.451392
O16	4.785668	-1.413521	-0.801275
N17	4.198558	0.652828	-0.015944
H18	5.187746	0.877233	-0.032858
C19	3.291856	1.574301	0.401782
N20	3.711228	2.771977	0.793710
H21	4.682614	3.042955	0.809624
H22	3.016626	3.436532	1.104784
N23	1.961110	1.350297	0.442749
C24	1.610491	0.143076	0.062086
C25	-3.249301	0.225709	-0.018136
H26	-4.005491	-0.163547	-0.710679
C27	-1.904811	0.432378	-0.721971
H28	-1.757785	-0.342735	-1.478719
H29	-1.828545	1.415230	-1.189670
O30	-3.690308	1.390704	0.632874
H31	-2.803113	-3.434016	-0.809370
H32	-3.999027	2.023951	-0.037381
O33	-4.448330	3.056894	-1.505986
H34	-4.407459	4.011220	-1.393833
H35	-5.276192	2.879839	-1.962644

dGuo$^{\bullet+}$·85′

O1	4.201733	1.140409	0.874779
C2	3.960799	-0.108988	1.513678
H3	3.619622	0.043558	2.543661

H4	4.878562	-0.709011	1.527230
C5	2.910387	-0.890325	0.758916
H6	2.879339	-1.903266	1.182044
O7	1.629542	-0.275523	0.930573
C8	0.859957	-0.643716	-0.183392
H9	0.456477	-1.658704	-0.076019
N10	-0.301374	0.239794	-0.218503
C11	-0.294837	1.604503	-0.285140
H12	0.637025	2.162877	-0.392752
N13	-1.521925	2.146144	-0.204503
C14	-2.337475	1.107517	-0.070753
C15	-3.790035	1.053076	0.064056
O16	-4.585470	1.953788	0.076954
N17	-4.227530	-0.302062	0.194513
H18	-5.232481	-0.397789	0.294816
C19	-3.429360	-1.400793	0.192008
N20	-3.972387	-2.605122	0.326856
H21	-4.963261	-2.758517	0.436661
H22	-3.354688	-3.404702	0.322850
N23	-2.086887	-1.348020	0.055608
C24	-1.608737	-0.131481	-0.064029
C25	3.126279	-1.045357	-0.768010
H26	3.974738	-0.445051	-1.110449
C27	1.808083	-0.531994	-1.373866
H28	1.913429	0.516028	-1.668192
H29	1.489759	-1.128599	-2.230635
O30	3.350408	-2.422267	-1.000891
H31	4.906520	1.603273	1.336262
H32	3.750870	-2.547398	-1.865886
O33	2.481089	2.605052	-0.748731
H34	2.862941	3.447014	-1.008247
H35	3.103089	2.178827	-0.131432

Guo$^{\bullet+}$·W12a

O1	-3.642262	1.912982	0.401736
C2	-4.301752	1.282933	-0.689241
H3	-4.179510	1.867047	-1.608890
H4	-5.374207	1.165286	-0.487036
C5	-3.694145	-0.091973	-0.901368
H6	-4.223207	-0.582182	-1.725139
O7	-2.316226	0.045629	-1.295009
C8	-1.464334	-0.522958	-0.347602
H9	-1.009203	-1.452353	-0.706390
N10	-0.356968	0.408463	-0.121366
C11	-0.467981	1.742832	0.128760
H12	-1.442943	2.215755	0.179633
N13	0.709827	2.359917	0.294645
C14	1.611628	1.392941	0.146279
C15	3.070872	1.434988	0.221059
O16	3.782385	2.381238	0.442391
N17	3.619392	0.146110	-0.009578
H18	4.639851	0.075828	0.024906
C19	2.911903	-0.982755	-0.272159
N20	3.571644	-2.112674	-0.475893
H21	4.587286	-2.140134	-0.435664
H22	3.036695	-2.948178	-0.662677
N23	1.558393	-1.029110	-0.338571
C24	0.982567	0.128780	-0.125830
C25	-3.691198	-1.003755	0.335870
H26	-4.484268	-0.749297	1.045269
C27	-2.297533	-0.770125	0.930124
H28	-2.315549	0.144365	1.528743
O29	-3.727089	-2.375065	-0.017282
H30	-4.112762	2.715373	0.644424
H31	-4.632044	-2.689276	-0.089247
O32	6.254686	-1.045415	-0.120090
H33	6.875517	-0.844819	-0.829158
H34	6.788082	-1.157332	0.674550
O35	-1.807724	-1.802515	1.721149
H36	-2.180083	-2.629307	1.383492

Guo$^{\bullet+}$·W16

O1	3.461817	-2.105376	0.453188
C2	4.198561	-1.543460	-0.625597
H3	4.047790	-2.122702	-1.544109
H4	5.272193	-1.517210	-0.398732
C5	3.716642	-0.123487	-0.861605
H6	4.302750	0.311004	-1.677803
O7	2.339744	-0.146840	-1.283531
C8	1.521850	0.503095	-0.359656
H9	1.157165	1.465721	-0.734251
N10	0.332295	-0.326341	-0.149864
C11	0.322383	-1.664127	0.104047
H12	1.252360	-2.219596	0.165666
N13	-0.907481	-2.175095	0.259349
C14	-1.718088	-1.132579	0.101224
C15	-3.174052	-1.038485	0.157362
O16	-3.972419	-1.921668	0.362069
N17	-3.607146	0.291092	-0.068612
H18	-4.635440	0.401726	-0.016358
C19	-2.801326	1.342945	-0.336428
N20	-3.345179	2.533312	-0.560579
H21	-4.342839	2.683202	-0.563626
H22	-2.729114	3.310324	-0.751942
N23	-1.448512	1.272280	-0.391267
C24	-0.977015	0.070533	-0.167843
C25	3.765308	0.797888	0.367565
H26	4.521127	0.486213	1.094588
C27	2.345678	0.685500	0.935087
H28	2.274119	-0.224028	1.537167
O29	3.919634	2.158016	0.004274
H30	3.857222	-2.941930	0.713949
H31	4.848274	2.397632	-0.051498
O32	-6.317514	-0.045074	0.089641
H33	-7.165909	0.268064	0.415112
H34	-6.287130	-0.999125	0.234309
O35	1.929015	1.760515	1.710869
H36	2.377736	2.550454	1.377334

Guo$^{\bullet+}$·W2b

O1	3.559244	-1.894915	0.219461
C2	4.138630	-1.121448	-0.823466

H3	4.036101	-1.630424	-1.789051
H4	5.204215	-0.939334	-0.633176
C5	3.422734	0.214995	-0.899822
H6	3.895752	0.816777	-1.682596
O7	2.050759	0.007840	-1.284528
C8	1.178956	0.411388	-0.272112
H9	0.642384	1.330650	-0.530360
N10	0.155494	-0.624619	-0.118695
C11	0.378906	-1.962371	0.004535
H12	1.389301	-2.357063	-0.002313
N13	-0.741433	-2.687000	0.125272
C14	-1.720623	-1.787688	0.077558
C15	-3.167499	-1.958276	0.161157
O16	-3.802513	-2.970669	0.299481
N17	-3.822045	-0.697540	0.053553
H18	-4.832860	-0.757648	0.108787
C19	-3.217860	0.514272	-0.107900
N20	-3.955010	1.604706	-0.198137
H21	-4.962596	1.572121	-0.150876
H22	-3.507112	2.525900	-0.311786
N23	-1.871652	0.665577	-0.181063
C24	-1.203271	-0.456490	-0.082781
C25	3.376489	1.007199	0.416108
H26	4.204542	0.756109	1.085685
C27	2.021459	0.603681	1.008791
H28	2.129012	-0.358344	1.516137
O29	3.292375	2.403819	0.192302
H30	4.095854	-2.676404	0.379029
H31	4.167655	2.794989	0.130845
O32	-3.079262	4.235283	-0.495089
H33	-2.940297	4.707787	-1.320758
H34	-2.835323	4.835870	0.214921
O35	1.471212	1.514177	1.903844
H36	1.773833	2.395294	1.642822

Guo$^{\bullet+}$·W3′

O1	2.322411	-2.556210	0.473925
C2	3.149248	-2.072966	-0.579053
H3	2.959168	-2.628193	-1.505350
H4	4.211647	-2.169976	-0.322363
C5	2.841641	-0.606276	-0.814390
H6	3.490773	-0.239809	-1.615330
O7	1.476880	-0.467606	-1.262518
C8	0.727199	0.267913	-0.347766
H9	0.475363	1.265630	-0.722387
N10	-0.552421	-0.428893	-0.156398
C11	-0.710113	-1.761103	0.073114
H12	0.152095	-2.418380	0.123648
N13	-1.991223	-2.134822	0.225406
C14	-2.678418	-1.006618	0.090756
C15	-4.115129	-0.759494	0.158103
O16	-5.009682	-1.537367	0.357357
N17	-4.392142	0.626085	-0.054657
H18	-5.379309	0.855869	-0.013646
C19	-3.469690	1.595012	-0.291968
N20	-3.869663	2.847483	-0.477646
H21	-4.836807	3.132293	-0.450922
H22	-3.160436	3.548539	-0.640434
N23	-2.140721	1.365344	-0.353328
C24	-1.806790	0.111377	-0.158514
C25	2.976007	0.302675	0.417424
H26	3.677953	-0.106298	1.151860
C27	1.543922	0.357215	0.961221
H28	1.348538	-0.530051	1.569378
O29	3.301380	1.627373	0.069966
H30	2.629137	-3.423391	0.752736
H31	4.267566	1.712102	-0.023294
O32	6.047553	1.532998	-0.179189
H33	6.481978	1.847947	-0.977555
H34	6.626814	1.766204	0.552536
O35	1.248546	1.488602	1.713839
H36	1.834736	2.192404	1.396878

Guo$^{\bullet+}$·W85′

O1	-4.147352	1.410930	-0.990755
C2	-3.916132	0.193783	-1.688839
H3	-3.579197	0.390500	-2.712569
H4	-4.834184	-0.405449	-1.725605
C5	-2.859382	-0.615913	-0.974733
H6	-2.807248	-1.600889	-1.461467
O7	-1.591625	0.033854	-1.090447
C8	-0.776362	-0.542251	-0.110329
H9	-0.399138	-1.531047	-0.405365
N10	0.394362	0.305996	0.049821
C11	0.404369	1.642176	0.333062
H12	-0.525539	2.188850	0.492076
N13	1.640785	2.162863	0.395578
C14	2.446923	1.138355	0.144339
C15	3.903653	1.072214	0.076849
O16	4.711525	1.946966	0.239458
N17	4.327872	-0.257940	-0.231254
H18	5.335492	-0.361484	-0.286806
C19	3.514638	-1.325477	-0.439297
N20	4.046572	-2.508785	-0.722290
H21	5.039956	-2.669157	-0.791753
H22	3.417441	-3.286780	-0.862986
N23	2.167360	-1.261955	-0.374814
C24	1.702132	-0.069056	-0.089323
C25	-3.074694	-0.863927	0.533392
H26	-3.779738	-0.146676	0.958778
C27	-1.656934	-0.668240	1.150487
H28	-1.627566	0.273018	1.705616
O29	-3.519326	-2.193744	0.717713
H30	-4.785098	1.944412	-1.472898
H31	-4.215430	-2.225196	1.379525
O32	-2.423328	2.459489	0.931895
H33	-2.810157	3.205081	1.397646
H34	-3.034593	2.220171	0.212660
O35	-1.251229	-1.703587	1.988157
H36	-1.792249	-2.477858	1.772041

Guo$^{\bullet+}$·W2′3′

O1	-2.555535	-2.510526	-0.561497
C2	-3.232813	-2.256576	0.661688
H3	-2.934394	-2.981953	1.427663
H4	-4.320730	-2.313441	0.527684
C5	-2.877116	-0.862295	1.148337
H6	-3.418260	-0.690584	2.086263
O7	-1.473137	-0.794526	1.450283
C8	-0.832387	0.121196	0.614826
H9	-0.538899	1.035125	1.140359
N10	0.409969	-0.499575	0.141814
C11	0.523928	-1.737978	-0.412756
H12	-0.351007	-2.366763	-0.542981
N13	1.780444	-2.064002	-0.752136
C14	2.498499	-1.001674	-0.404464
C15	3.930689	-0.747867	-0.523295
O16	4.790632	-1.455275	-0.976162
N17	4.252082	0.543059	-0.002118
H18	5.237932	0.774269	-0.063188
C19	3.370630	1.425901	0.536231
N20	3.808816	2.594089	0.989868
H21	4.776752	2.875771	0.958035
H22	3.127736	3.235053	1.372751
N23	2.045603	1.189943	0.644250
C24	1.671508	0.023114	0.176309
C25	-3.159535	0.279705	0.154207
H26	-3.939753	0.012077	-0.566717
C27	-1.794248	0.448913	-0.534162
H28	-1.728815	-0.346423	-1.290243
O29	-3.482912	1.494750	0.813457
H30	-2.895407	-3.318443	-0.956449
H31	-4.255206	1.359311	1.371771
O32	-3.932352	2.586245	-1.744618
O33	-1.458226	1.690316	-1.054185
H34	-2.216128	2.059887	-1.545917
H35	-4.070647	2.708070	-0.794906
H36	-4.254252	3.370940	-2.195607

Cartesian coordinates for the structures in Fig. 5, optimized at ωB97XD/6-31+G(d,p).

9HG$^{\bullet+}$_keto

C1	-0.246525	1.479497	0.000004
C2	0.854816	0.518755	0.000002
H3	-2.305573	1.419067	0.000005
C4	-1.679426	-0.548633	0.000006
C5	2.692392	-0.514115	-0.000013
N6	-1.503772	0.796299	0.000005
N7	2.171493	0.715558	-0.000015
N8	1.751847	-1.500377	0.000006
N9	-0.652665	-1.437674	0.000017
C10	0.531203	-0.880468	0.000012
N11	-2.901167	-1.058213	-0.000036
H12	-2.995044	-2.065277	0.000073
H13	-3.739392	-0.495433	-0.000028
O14	-0.200466	2.678487	0.000007
H15	3.753107	-0.726499	-0.000026
H16	1.915718	-2.499117	0.000006

9HG$^{\bullet+}$_keto·W16

C1	-0.429751	-1.044077	-0.000001
C2	0.996756	-0.723291	-0.000001
H3	-2.237034	-0.053917	-0.000014
C4	-0.737314	1.396791	-0.000001
C5	3.104682	-0.679664	0.000000
N6	-1.217011	0.135122	-0.000007
N7	2.066610	-1.518154	0.000000
N8	2.741407	0.633767	0.000000
N9	0.588791	1.709892	0.000000
C10	1.371220	0.662598	-0.000001
N11	-1.581984	2.417484	0.000004
H12	-1.202138	3.354074	0.000008
H13	-2.584000	2.294865	0.000014
O14	-0.945371	-2.134143	0.000003
H15	4.140416	-0.991647	0.000001
H16	3.356929	1.436604	0.000001
O17	-3.720634	-0.940987	0.000014
H18	-4.680018	-0.883441	-0.000121
H19	-3.484362	-1.876415	0.000030

water-assisted TS

C1	1.353054	0.650023	0.006672
C2	0.891686	-0.705081	0.002081
C3	-0.549988	-0.904648	-0.003364
N4	-1.305904	0.248283	0.012458
C5	-0.724994	1.459845	0.002131
N6	0.625999	1.730345	0.006446
N7	2.722638	0.533542	0.007848
C8	2.998142	-0.798977	0.002956
N9	1.908410	-1.570145	-0.000587
O10	-1.088418	-2.022812	-0.021174
H11	4.010765	-1.179201	0.002022
N12	-1.496929	2.541254	-0.012053
H13	-2.502119	2.472434	-0.045691
H14	-1.061785	3.452641	-0.024206
H15	3.389435	1.293890	0.008708
H16	-2.728962	-0.275838	0.014351
O17	-3.358310	-1.136627	-0.070386
H18	-2.549581	-1.811810	-0.050637
H19	-3.970828	-1.266530	0.666276

TS (no water)

C1	-0.343249	1.369789	0.000186
C2	0.854464	0.577088	0.000109
H3	-1.818639	1.985859	0.000184
C4	-1.633678	-0.636593	-0.000111
C5	2.746413	-0.347727	0.000007
N6	-1.531133	0.702410	0.000074
N7	2.157055	0.853423	0.000167
N8	1.870570	-1.385192	-0.000157
N9	-0.536236	-1.470634	-0.000213
C10	0.606102	-0.844505	-0.000099
N11	-2.817769	-1.219876	-0.000211
H12	-2.868855	-2.229601	-0.000368
H13	-3.670605	-0.678106	-0.000148
O14	-0.616966	2.589990	0.000307
H15	3.818118	-0.495778	0.000003
H16	2.097990	-2.371524	-0.000303

9HG$^{\bullet+}$_enol·W6

C1	0.706519	-0.502708	0.021542
C2	-0.712806	-0.791376	0.008890
H3	4.593538	-0.749644	0.726199
C4	0.162735	1.733927	0.002018
C5	-2.685085	-1.536345	-0.006434
N6	1.096544	0.756087	0.022683
N7	-1.408904	-1.931034	0.008096
N8	-2.839560	-0.186063	-0.015254
N9	-1.210160	1.602138	-0.010562
C10	-1.573726	0.353313	-0.005809
N11	0.603717	2.981955	-0.007852
H12	-0.054079	3.748932	-0.024639
H13	1.598230	3.161600	-0.007304
O14	1.536075	-1.487274	0.033803
H15	-3.528274	-2.213884	-0.010821
H16	-3.710566	0.327677	-0.027037
O17	4.077318	-0.965030	-0.056741
H18	4.614050	-1.554254	-0.596656
H19	2.502674	-1.204452	0.022748

9HG$^{\bullet+}$_enol

C1	-0.372887	1.332424	-0.000003
C2	0.800774	0.493895	-0.000003
C3	-1.656236	-0.574521	0.000006
C4	2.680229	-0.458597	-0.000006
N5	-1.560826	0.781169	0.000002
N6	2.109729	0.751019	-0.000007
N7	1.788705	-1.483340	-0.000001
N8	-0.630503	-1.490286	0.000006

C9	0.536193	-0.915212	0.000001
N10	-2.874420	-1.085256	0.000011
H11	-3.000036	-2.088901	0.000013
H12	-3.678960	-0.472296	0.000012
O13	-0.218106	2.625883	-0.000007
H14	3.749442	-0.623487	-0.000008
H15	1.998901	-2.473098	0.000001
H16	-1.081726	3.069639	-0.000006

Cartesian coordinates for the structures in Fig. 6, optimized at ωB97XD/6-31+G(d,p).

9HG$^{\bullet+}$

C1	-0.246525	1.479497	0.000004
C2	0.854816	0.518755	0.000002
H3	-2.305573	1.419067	0.000005
C4	-1.679426	-0.548633	0.000006
C5	2.692392	-0.514115	-0.000013
N6	-1.503772	0.796299	0.000005
N7	2.171493	0.715558	-0.000015
N8	1.751847	-1.500377	0.000006
N9	-0.652665	-1.437674	0.000017
C10	0.531203	-0.880468	0.000012
N11	-2.901167	-1.058213	-0.000036
H12	-2.995044	-2.065277	0.000073
H13	-3.739392	-0.495433	-0.000028
O14	-0.200466	2.678487	0.000007
H15	3.753107	-0.726499	-0.000026
H16	1.915718	-2.499117	0.000006

9HG$^{\bullet+}$·W

C1	-0.235186	1.386170	-0.496027
C2	0.869041	0.437303	-0.385743
H3	-2.288017	1.320063	-0.540630
C4	-1.656460	-0.625374	-0.279724
C5	2.707871	-0.572730	-0.204491
N6	-1.485010	0.703088	-0.481417
N7	2.184875	0.642261	-0.373768
N8	1.769640	-1.558433	-0.104233
N9	-0.633136	-1.506413	-0.156677
C10	0.549032	-0.951008	-0.212740
N11	-2.880906	-1.128893	-0.209039
H12	-2.975550	-2.126843	-0.080147
H13	-3.716961	-0.569624	-0.288533
O14	-0.188787	2.583351	-0.592962
H15	3.768312	-0.778504	-0.151034
O16	-0.143212	0.557265	2.342061
H17	0.174657	1.412965	2.648925
H18	-0.336528	0.057008	3.140547
H19	1.936057	-2.547425	0.026355

9HG$^{\bullet+}$·2W

C1	0.077789	1.055505	0.927226
C2	-0.475097	-0.273597	0.691760
H3	1.868065	2.019609	0.648895
C4	2.130694	0.098317	-0.055492
C5	-1.667828	-1.990860	0.425240
N6	1.442619	1.105822	0.536580
N7	-1.710537	-0.738928	0.882670
N8	-0.443050	-2.351395	-0.049433
N9	1.620655	-1.138551	-0.270566
C10	0.370660	-1.260352	0.086758
N11	3.383223	0.297201	-0.440532
H12	3.873733	-0.474587	-0.870915
H13	3.861680	1.179680	-0.339165
O14	-0.473770	2.018589	1.392316
H15	-2.509024	-2.670438	0.424117
O16	-0.504692	0.643536	-1.909828
H17	-3.029132	1.021909	0.026676
H18	-0.443292	0.639401	-2.868239
H19	-0.187399	-3.239772	-0.459653
O20	-2.943040	1.374391	-0.867133
H21	-1.394086	0.987303	-1.690649
H22	-3.336200	2.251642	-0.857890

TS1·W

C1	-0.695172	1.475590	-0.058911
C2	0.410628	0.558655	-0.242194
H3	-2.732076	1.355220	0.194939
C4	-2.050124	-0.594983	0.089494
C5	2.359515	-0.479463	-0.417326
N6	-1.919800	0.758291	0.082775
N7	1.718277	0.811803	-0.416545
N8	1.366907	-1.458842	-0.286031
N9	-1.007236	-1.436275	-0.015964
C10	0.152618	-0.840861	-0.172225
N11	-3.260833	-1.132270	0.217015
H12	-3.331847	-2.139473	0.225928
H13	-4.104354	-0.586485	0.298153
O14	-0.676992	2.681657	-0.024813
H15	3.128932	-0.671481	-1.164398
O16	3.113401	-0.144274	0.907113
H17	2.618255	0.887266	0.645063
H18	4.083539	-0.201933	0.864458
H19	1.500275	-2.454767	-0.384324

TS1·2W

C1	0.822723	1.442696	0.251264
C2	-0.089196	0.330084	0.402271
H3	2.814347	1.720909	-0.168302
C4	2.493070	-0.323038	-0.232781
C5	-1.800503	-1.014992	0.639005
N6	2.131010	0.979855	-0.062218
N7	-1.384819	0.338032	0.721232
N8	-0.663453	-1.809134	0.350405
N9	1.635841	-1.344176	-0.132276
C10	0.403739	-0.982721	0.173795
N11	3.766824	-0.603194	-0.521189
H12	4.019124	-1.572034	-0.646246
H13	4.481002	0.100613	-0.614640
O14	0.591526	2.626650	0.354797
H15	-2.412528	-1.373228	1.468710
O16	-2.788418	-1.048620	-0.576631
H17	-2.667629	1.525614	-0.118830
H18	-3.462577	-1.738796	-0.500759
H19	-0.618059	-2.816638	0.367997
O20	-3.323049	1.268450	-0.810234
H21	-3.199455	0.035357	-0.756279
H22	-4.171523	1.704505	-0.668107

[8-OH-9HG + H]$^{\bullet+}$

C1	0.807780	1.466867	0.000120
C2	-0.348310	0.625481	0.152319
H3	2.836623	1.220552	-0.199907
C4	2.021148	-0.682284	-0.059645
C5	-2.470098	-0.290208	0.308059
N6	1.983957	0.681870	-0.094869
N7	-1.645993	0.926317	0.286659
N8	-1.430980	-1.312860	0.333409
N9	0.932898	-1.451555	0.076548
C10	-0.204799	-0.793273	0.179986
N11	3.198082	-1.293166	-0.165871
H12	3.208468	-2.302722	-0.139946
H13	4.071672	-0.802919	-0.277639
O14	0.836244	2.677103	-0.046268
H15	-3.073181	-0.319457	1.222437
O16	-3.245768	-0.399906	-0.826164
H17	-2.038137	1.853217	0.182835
H18	-4.185681	-0.381220	-0.616938
H19	-1.643644	-2.298765	0.272440

[8-OH-9HG + H]$^{\bullet+}$·W

C1	-0.508494	1.374975	0.042606
C2	0.252134	0.167577	-0.115447
H3	-2.478580	1.911099	0.216555
C4	-2.440850	-0.157457	0.042669
C5	1.866073	-1.467526	-0.296165
N6	-1.890397	1.092266	0.109787
N7	1.567780	-0.034011	-0.220161
N8	0.522687	-2.028873	-0.347690
N9	-1.723690	-1.275108	-0.105430
C10	-0.418250	-1.089886	-0.183879
N11	-3.764797	-0.275055	0.127627
H12	-4.158170	-1.203569	0.076070
H13	-4.387177	0.508396	0.246887
O14	-0.095989	2.519207	0.116204
H15	2.421763	-1.682241	-1.216402
O16	2.523975	-1.936295	0.823616
H17	2.266709	0.729861	-0.166784
H18	3.456153	-2.095748	0.641344
H19	0.352235	-3.023658	-0.304023
O20	2.766835	2.382664	-0.132194
H21	3.519992	2.904431	0.155769
H22	1.963741	2.906185	0.001930

TS2

C1	0.840735	1.467061	-0.010457
C2	-0.312812	0.611231	-0.043946
H3	2.870181	1.205211	0.006992
C4	2.049386	-0.704225	-0.005386
C5	-2.345159	-0.261367	0.066572
N6	2.009198	0.669881	-0.009119
N7	-1.662050	0.899103	-0.043395
N8	-1.448049	-1.279059	-0.002593
N9	0.961819	-1.463272	-0.006675
C10	-0.169798	-0.760610	-0.027101
N11	3.248351	-1.296969	0.004197
H12	3.276220	-2.305319	0.005224
H13	4.118016	-0.789720	-0.000779
O14	0.876780	2.676779	0.008235
H15	-2.500455	-0.171676	1.943261
O16	-3.616785	-0.486248	-0.208391
H17	-2.063039	1.828831	-0.065751
H18	-4.221306	0.147567	0.199261
H19	-1.698575	-2.259474	0.038048

TS2·W

C1	0.606639	1.353720	-0.011577
C2	-0.208637	0.178298	-0.046554
H3	2.604049	1.776844	0.009941
C4	2.453918	-0.297756	-0.007010
C5	-1.842758	-1.289343	0.068747
N6	1.965777	0.989382	-0.010148
N7	-1.579284	0.023483	-0.047826
N8	-0.665228	-1.975386	-0.006414
N9	1.675168	-1.368044	-0.008735
C10	0.374492	-1.073556	-0.028856
N11	3.782572	-0.462029	0.002254
H12	4.140322	-1.405084	0.004062
H13	4.436947	0.302812	-0.002056
O14	0.260905	2.523950	0.010483
H15	-1.991720	-1.242995	1.906331
O16	-2.975045	-1.919753	-0.189180
H17	-2.233278	0.842884	-0.052464
H18	-3.754017	-1.431497	0.107358
H19	-0.587879	-2.983084	0.045578
O20	-2.567456	2.458330	0.042810
H21	-3.218595	3.065226	-0.318497
H22	-1.698015	2.894660	0.034439

TS3

C1	-0.849234	1.466252	0.002758
C2	0.326174	0.627267	-0.022648
H3	-2.885486	1.206977	0.032006
C4	-2.049835	-0.691334	0.012018
C5	2.419636	-0.276407	-0.105639
N6	-2.022854	0.672687	0.015046
N7	1.631600	0.922400	-0.011422
N8	1.442226	-1.301050	-0.023429
N9	-0.942356	-1.456612	-0.010420
C10	0.189739	-0.794359	-0.024874
N11	-3.219387	-1.315443	0.029967
H12	-3.215141	-2.326457	0.029218
H13	-4.107348	-0.836741	0.049948
O14	-0.885448	2.673652	0.014400
H15	2.750697	-0.249628	-1.569557
O16	3.601913	-0.383435	0.381834
H17	2.047878	1.845173	0.044128
H18	3.540158	-0.323747	-0.954952
H19	1.694027	-2.279711	0.031452

8-OH-9HG^{+}

C1	-0.803512	1.467332	-0.000001
C2	0.339501	0.604898	-0.000034
H3	-2.834826	1.213418	0.000033
C4	-2.024900	-0.699771	0.000003
C5	2.362630	-0.275584	-0.000004
N6	-1.976784	0.673319	0.000012
N7	1.708805	0.883701	-0.000024
N8	1.478154	-1.286299	0.000013
N9	-0.940472	-1.462253	0.000000
C10	0.190489	-0.756584	-0.000012
N11	-3.228263	-1.287342	-0.000006
H12	-3.261519	-2.295238	-0.000006
H13	-4.094799	-0.775213	0.000011
O14	-0.838402	2.678275	0.000019
O15	3.648241	-0.510553	0.000005
H16	2.110417	1.812978	-0.000085
H17	4.201652	0.281111	0.000135
H18	1.725023	-2.268475	0.000035

8-OH-9HG^{+}·W

C1	-0.567401	1.344615	0.007860
C2	0.229294	0.161662	0.012679
H3	-2.559961	1.790719	-0.000775
C4	-2.435687	-0.285103	-0.001818
C5	1.841785	-1.320631	0.002833
N6	-1.931607	0.995164	0.003488
N7	1.612743	-0.018400	0.013542
N8	0.673651	-1.996149	-0.001163
N9	-1.668314	-1.362981	-0.002543
C10	-0.365246	-1.075633	0.003666
N11	-3.767637	-0.433716	-0.006670
H12	-4.136945	-1.372028	-0.012028
H13	-4.412147	0.339215	-0.007680
O14	-0.211911	2.513863	0.006323
O15	2.981735	-1.963669	-0.001129
H16	2.274577	0.794094	0.022099
H17	3.751666	-1.380620	-0.023177
H18	0.587037	-3.004414	-0.011691
O19	2.590537	2.413621	-0.052123
H20	3.250641	3.047265	0.239562
H21	1.713932	2.838353	-0.028782

8O-9HG$^{\bullet+}$

C1	-0.757104	1.466819	0.000005
C2	0.408564	0.612986	0.000003
H3	-2.796167	1.233224	-0.000055
C4	-1.983858	-0.675768	0.000011
C5	2.474613	-0.310180	0.000000
N6	-1.939937	0.688282	0.000020
N7	1.718933	0.892552	-0.000001
N8	1.502359	-1.329379	0.000003
N9	-0.885611	-1.455162	0.000011
C10	0.255021	-0.808086	0.000001
N11	-3.160663	-1.285072	-0.000130
H12	-3.169152	-2.296182	0.000246
H13	-4.042955	-0.795344	0.000439
O14	-0.776689	2.674306	-0.000006
O15	3.662986	-0.416118	-0.000001
H16	1.742572	-2.312713	0.000000
H17	2.146346	1.812335	-0.000007

8O-9HG$^{\bullet+}$ (*enol*)

C1	-0.763137	1.480362	0.000002
C2	0.421160	0.629856	-0.000008
H3	-2.804604	1.227401	0.000003
C4	-1.997772	-0.674809	0.000000
C5	2.341145	-0.226048	0.000014
N6	-1.948203	0.682716	-0.000021
N7	1.715991	0.953602	-0.000007
N8	1.501260	-1.304176	0.000005
N9	-0.895487	-1.458533	0.000011
C10	0.230173	-0.792369	0.000010
N11	-3.172114	-1.290529	0.000009
H12	-3.177027	-2.301446	-0.000022
H13	-4.055863	-0.803355	-0.000097
O14	-0.828048	2.680565	0.000018
O15	3.624817	-0.413507	-0.000015
H16	4.092478	0.437069	-0.000035
H17	1.771319	-2.279643	0.000041