Scheme 1. $GW^{\bullet+}$, B3LYP/6-31+G(d)

Electronic energy =-894.1553709 hartree

7	4.355110	-1.649479	-0.730424
1	4.742369	-1.670710	-1.668752
6	3.091839	-2.368971	-0.622216
6	1.897074	-1.426639	-0.402157
1	2.856043	-2.968243	-1.509730
1	3.097805	-3.064043	0.225383
8	0.736762	-1.871401	-0.369990
7	2.214000	-0.131444	-0.238138
1	3.214701	0.087870	-0.277288
6	1.271110	0.941475	-0.017082
1	0.619451	1.052990	-0.894689
6	0.351937	0.739882	1.243918
6	2.085330	2.234348	0.111461
1	0.960153	0.319166	2.050832
1	0.016148	1.731509	1.565032
6	-0.845562	-0.107246	0.980499
8	3.289361	2.293106	0.031639
6	-1.062149	-1.433917	1.459091
6	-2.007085	0.229655	0.222322
1	-0.415836	-2.040049	2.078119
7	-2.242521	-1.882839	1.026297
6	-2.877206	-0.893405	0.251117
6	-2.401354	1.384345	-0.486402
1	-2.624851	-2.798613	1.231583
6	-4.102354	-0.912651	-0.386063
6	-3.636263	1.380113	-1.135240
1	-1.760194	2.260308	-0.528628
1	-4.759110	-1.777024	-0.357083
6	-4.471817	0.253126	-1.086527
1	-3.958019	2.258349	-1.685812
1	-5.428269	0.275144	-1.600035
8	1.284514	3.297404	0.321056
1	1.844402	4.094991	0.396286
1	5.062989	-1.988881	-0.087321

Scheme 1. Structure II. B3LYP/6-31+G(d)

Electronic energy = -894.1339673 hartree

7	3.430805	-2.654235	-0.804237
1	3.698342	-3.478531	-0.273720
6	4.308033	-1.511812	-0.521338

6	3.537611	-0.214549	-0.249297
1	4.916856	-1.699603	0.369826
1	5.009501	-1.290861	-1.333862
8	4.168566	0.842778	-0.111424
7	2.197150	-0.368606	-0.172780
1	1.945661	-1.341438	-0.376528
6	1.072361	0.551627	0.018748
1	0.465200	0.491248	-0.892169
6	0.188112	0.039432	1.232214
6	1.260476	2.096093	0.196736
1	0.792980	-0.642733	1.836059
1	-0.057827	0.906666	1.854287
6	-1.089018	-0.619691	0.835538
8	0.221856	2.721495	0.332014
6	-1.399169	-2.000503	1.017716
6	-2.239047	-0.043457	0.214257
1	-0.786743	-2.777740	1.457371
7	-2.627819	-2.256404	0.549812
6	-3.197616	-1.077250	0.036721
6	-2.551120	1.267942	-0.215094
1	-3.077688	-3.165662	0.564558
6	-4.432086	-0.866764	-0.540081
6	-3.805608	1.495648	-0.802308
1	-1.827367	2.069401	-0.086906
1	-5.159536	-1.662749	-0.670079
6	-4.724983	0.457721	-0.960664
1	-4.062103	2.495431	-1.137570
1	-5.689477	0.657218	-1.417650
8	2.434842	2.666382	0.186100
1	3.205167	2.013893	0.052178
1	3.456287	-2.911701	-1.787774

Scheme 1. TS (II-III). B3LYP/6-31+G(d)

Electronic energy = -894.109974 hartree

7	-4.247689	-2.048518	-0.688031
1	5.000816	-1.895603	-1.352830
6	-4.407322	-1.245962	0.520812
6	-3.241867	-0.294505	0.685434
1	-5.321086	-0.638972	0.509040
1	-4.460311	-1.853974	1.433538
8	-3.262844	0.492232	1.720488
7	-2.280085	-0.319849	-0.213682
1	-2.525680	-0.965362	-0.980043

6	-1.034906	0.368996	-0.225320
1	-0.600817	0.432349	0.773816
6	-0.080996	-0.024445	-1.347695
6	-1.374531	2.413035	-0.295411
1	-0.599678	-0.660624	-2.076351
1	0.236809	0.872419	-1.889181
6	1.089417	-0.731257	-0.745958
8	-0.748449	2.853840	-1.203037
6	1.197827	-2.099359	-0.471402
6	2.311141	-0.126763	-0.282664
1	0.501352	-2.901501	-0.678349
7	2.402574	-2.354199	0.103153
6	3.123273	-1.167118	0.237940
6	2.800047	1.193278	-0.279483
1	2.743516	-3.273838	0.352242
6	4.396527	-0.940828	0.751654
6	4.073743	1.431052	0.237130
1	2.203167	2.012352	-0.671738
1	5.013327	-1.747655	1.137195
6	4.859033	0.380931	0.744999
1	4.468263	2.442464	0.245659
1	5.848207	0.596207	1.137692
8	-2.110327	2.581418	0.657339
1	-2.717815	1.321756	1.562022
1	-4.207419	-3.044309	-0.491339

Scheme 1. Structure III. B3LYP/6-31+G(d)

Electronic energy = -894.1449734 hartree

7	-0.582141	2.701509	-0.914770
1	-0.881955	3.197432	-1.748062
6	0.824296	2.926256	-0.604887
6	1.518422	1.603252	-0.373943
1	1.341065	3.433960	-1.429510
1	0.988697	3.548550	0.285728
8	2.785607	1.667330	-0.025137
7	0.820567	0.484210	-0.528482
1	-0.158571	0.702023	-0.803637
6	1.162882	-0.820394	-0.362920
1	2.180883	-1.053744	-0.071362
6	0.156526	-1.908010	-0.600631
6	5.688344	-0.759068	0.764106
1	0.470787	-2.482156	-1.487492
1	0.242424	-2.619711	0.236162

6	-1.260161	-1.437971	-0.764395
8	6.787919	-1.011282	1.030541
6	-2.017055	-1.500933	-1.915179
6	-2.108810	-0.867005	0.258125
1	-1.756498	-1.885718	-2.892765
7	-3.274136	-0.999949	-1.671927
6	-3.366871	-0.603615	-0.349529
6	-1.934053	-0.562819	1.622916
1	-4.027179	-0.974433	-2.344966
6	-4.437904	-0.043404	0.357236
6	-2.995639	-0.008385	2.329641
1	-0.993085	-0.774195	2.126811
1	-5.395672	0.146534	-0.119867
6	-4.234056	0.251066	1.701427
1	-2.878716	0.218608	3.385565
1	-5.046314	0.678481	2.282118
8	4.568613	-0.511760	0.493202
1	3.248706	0.815748	0.116368
1	-1.200143	2.961228	-0.151011

Scheme 1. Structure IV. B3LYP/6-31+G(d)

Electronic energy =-705.5445333 hartree

7	1.483628	-1.694577	1.502107
1	1.492244	-1.811096	2.510391
6	2.823553	-1.645954	0.931940
6	2.947730	-0.437343	0.033820
1	3.592287	-1.563589	1.711149
1	3.086310	-2.532319	0.337784
8	4.098522	-0.292393	-0.598234
7	1.915801	0.390044	-0.074895
1	1.123790	0.063739	0.517196
6	1.741080	1.512251	-0.818788
1	2.560912	1.851352	-1.445654
6	0.450273	2.275159	-0.769092
1	0.650223	3.260355	-0.317495
1	0.165422	2.499340	-1.809948
6	-0.664714	1.585296	-0.038337
6	-1.245372	1.997167	1.142929
6	-1.364136	0.387386	-0.448361
1	-1.025804	2.862231	1.755374
7	-2.252889	1.130043	1.490977
6	-2.355843	0.132152	0.538093
6	-1.261785	-0.482506	-1.552446

1	-2.856184	1.236759	2.294508
6	-3.229094	-0.959302	0.458498
6	-2.128000	-1.567107	-1.636467
1	-0.534748	-0.302323	-2.341839
1	-3.986209	-1.137154	1.217513
6	-3.099761	-1.804136	-0.638923
1	-2.069474	-2.237169	-2.489575
1	-3.766610	-2.655749	-0.737281
1	4.159412	0.499812	-1.161724
1	0.910887	-2.431995	1.100957

Scheme 1. Structure TS(IV-V). B3LYP/6-31+G(d)

Electronic energy =-705.517557 hartree

7	4.289287	1.671551	-0.826559
1	-4.681880	2.430628	-0.278158
6	-4.679415	0.361882	-0.308091
6	-3.467350	-0.511794	-0.126232
1	-5.169029	0.440829	0.670491
1	-5.381199	-0.181414	-0.953929
8	-3.560388	-1.743548	0.223859
7	-2.239084	-0.056218	-0.327961
1	-2.141995	0.888852	-0.698901
6	-1.219345	-1.074720	-0.131314
1	-0.685625	-1.311699	-1.051620
6	-0.366419	-0.990562	1.136917
1	-0.974910	-0.679772	1.991664
1	0.051031	-1.975258	1.366948
6	0.712733	-0.011039	0.817284
6	0.643184	1.383855	0.966919
6	2.004313	-0.288179	0.230769
1	-0.148999	1.990487	1.386097
7	1.801174	1.945127	0.540073
6	2.671447	0.953150	0.080037
6	2.666239	-1.468164	-0.147559
1	2.021885	2.931525	0.595966
6	3.964062	1.060008	-0.423949
6	3.960889	-1.374474	-0.660119
1	2.186413	-2.437914	-0.047017
1	4.466930	2.018141	-0.519199
6	4.599582	-0.129729	-0.797035
1	4.486298	-2.277233	-0.956156
1	5.608925	-0.088365	-1.194963
1	-2.416390	-1.989246	0.162275

1 -4.587489 1.804200 -1.788994

Scheme 1. Structure V. B3LYP/6-31+G(d)

Electronic energy = -705.583691 hartree

7	4.912840	-.082333	-.595421
1	5.304989	.163185	-1.500148
6	3.783000	-1.003542	-.711181
6	2.434985	-.312037	-.463761
1	3.712642	-1.492620	-1.690456
1	3.860906	-1.807626	.029381
8	1.365378	-.924835	-.617202
7	2.509321	.963344	-.041525
1	3.463751	1.311187	.061196
6	1.366615	1.806832	.253596
1	.754449	1.921779	-.648523
6	.460142	1.311461	1.425503
1	1.095914	.988105	2.256576
1	-.107386	2.183506	1.774411
6	-.497602	.236760	1.039541
6	-.378525	-1.150988	1.351399
6	-1.712292	.365422	.298997
1	.403181	-1.651747	1.905410
7	-1.417859	-1.819844	.846287
6	-2.281793	-.930464	.180033
6	-2.382219	1.461848	-.282005
1	-1.562137	-2.819007	.933361
6	-3.469376	-1.174313	-.481779
6	-3.583223	1.232764	-.954245
1	-1.976500	2.466876	-.211024
1	-3.894027	-2.170281	-.565490
6	-4.117704	-.061146	-1.052816
1	-4.113155	2.064253	-1.407807
1	-5.053908	-.213200	-1.581302
1	1.762041	2.789046	.522207
1	5.664052	-.458538	-.025251

Figure 4, structure I B3LYP/6-31+G(d)

Electronic energy = -837.5801913 hartree

6	0.225199	-0.796387	0.000000
6	1.638102	-1.291262	0.000000

8	2.587812	-0.508857	0.000000
1	-0.588889	-1.518986	0.000000
6	0.000000	0.553162	0.000000
6	-1.264897	1.196273	0.000000
1	0.889660	1.180615	0.000000
6	-2.557025	0.572349	0.000000
6	-1.519982	2.618612	0.000000
1	-2.812451	-0.478912	0.000000
7	-3.500432	1.512431	0.000000
6	-2.922530	2.798946	0.000000
1	-4.498352	1.325835	0.000000
6	-0.686087	3.748647	0.000000
6	-3.530249	4.042351	0.000000
1	-4.609455	4.163303	0.000000
6	-2.674617	5.160684	0.000000
1	-3.109358	6.155419	0.000000
6	-1.281087	5.015254	0.000000
1	0.395359	3.649837	0.000000
1	-0.652663	5.900127	0.000000
7	1.770602	-2.640249	0.000000
6	3.070417	-3.281506	0.000000
1	3.653806	-2.999588	0.884963
1	0.971364	-3.268044	0.000000
6	2.852171	-4.784337	0.000000
8	1.757561	-5.309703	0.000000
8	4.015747	-5.447122	0.000000
1	3.830541	-6.406542	0.000000
1	3.653806	-2.999588	-0.884963

Figure 7, structure VI, B3LYP/6-31+G(d)

Electronic energy = -700.2277417

7	5.119255	-.528061	-.423458
1	4.886042	-1.451619	-.073116
6	4.189080	.438832	-.465096
6	2.872160	.179524	-.033717
1	4.482394	1.412884	-.837667
8	2.624588	-.993720	.501936
7	1.885436	1.102845	-.169151
1	2.119784	1.950371	-.671694
6	.655678	1.141166	.633117
6	-.307597	-.005199	.303242
1	.904553	1.064308	1.700673
1	.195401	2.117340	.469577
8	.119015	-1.176804	.239701

7	-1.594437	.298045	.148948
1	-1.934361	1.257126	.191420
6	-2.625580	-.707130	-.073613
6	-3.956422	.018773	-.180077
1	-2.431433	-1.271606	-.992496
1	-2.654516	-1.428713	.750542
8	-4.066546	1.224383	-.092347
8	-4.963017	-.835535	-.379768
1	-5.799734	-.333709	-.442218
1	6.073107	-.356804	-.713509
1	1.610754	-1.211761	.464797

Figure 7, structure VII, B3LYP/6-31++G(d,p)

Electronic energy = -415.7485397 hartree

7	-2.699401	-0.763399	0.000013
1	-3.710965	-0.759440	-0.000202
6	-2.008844	0.383799	-0.000040
1	-2.560661	1.316189	-0.000038
6	-0.611815	0.395636	-0.000005
8	0.071558	-0.764057	0.000045
6	1.481248	-0.482766	-0.000087
8	2.287646	-1.344831	0.000029
6	1.609666	1.033738	0.000015
1	2.149369	1.369154	0.892645
1	2.149353	1.369308	-0.892559
7	0.214382	1.454719	0.000083
1	-0.093246	2.418558	-0.000366
1	-2.233880	-1.664346	-0.000034

Figure 7, structure VIII, B3LYP/6-31++G(d,p)

Electronic energy =-416.3676234 hartree

6	-0.617579	-1.637182	0.000000
6	0.900323	-1.508922	0.000000
8	1.159823	-0.053133	0.000000
6	0.000000	0.563390	0.000000
7	-1.029253	-0.238444	0.000000
1	-1.969473	0.161598	0.000000
1	-0.959454	-2.170204	0.893279
1	-0.959454	-2.170204	-0.893279

8	1.780053	-2.286361	0.000000
6	-0.118700	2.059575	0.000000
1	0.432534	2.427797	-0.875311
1	0.432534	2.427797	0.875311
7	-1.526570	2.420758	0.000000
1	-1.794600	2.950907	0.822298
1	-1.794600	2.950907	-0.822298

Figure 7, structure IX, B3LYP/6-31++G(d,p)

Electronic energy =-302.3910705 hartree

7	-2.349460	-0.128391	0.000000
1	-2.403513	0.888173	0.000000
6	-1.165053	-0.711192	0.000000
6	0.000000	0.122175	0.000000
1	-1.125535	-1.795980	0.000000
8	-0.010122	1.351417	0.000000
7	1.264508	-0.581942	0.000000
1	1.260649	-1.601434	0.000000
1	-3.211145	-0.659653	0.000000
6	2.405089	0.043504	0.000000
1	2.388103	1.129263	0.000000
1	3.326861	-0.526292	0.000000

Figure 7, structure X, B3LYP/6-31++G(d,p)

Electronic energy =-302.3517911 hartree

6	-1.282391	-0.818871	0.146417
7	-1.348505	0.705686	-0.101546
6	0.032282	1.180029	0.069903
6	0.934111	0.023523	0.004892
7	0.099111	-1.086060	-0.134550
1	0.476995	-2.026287	-0.111869
1	-1.976105	-1.323490	-0.528591
1	-1.686655	0.896478	-1.057659
8	2.144804	0.048561	0.022327
1	-2.009176	1.159922	0.541938
1	0.255415	2.237584	0.112453
1	-1.577158	-0.978160	1.190519

Figure 8. Structure XI, B3LYP/6-31+G(d)

Electronic energy =-700.1972767 hartree

7	3.934144	-1.921240	-0.222312
1	3.227111	-2.557769	0.128841
6	3.666130	-0.601671	-0.280072
6	2.371199	-0.142934	0.082009
1	4.453648	0.065736	-0.608997
8	1.477324	-0.944942	0.504266
7	2.081748	1.205490	-0.045616
1	2.782316	1.822822	-0.436257
6	0.971125	1.831971	0.656452
6	-0.348120	1.553953	-0.066895
1	0.914750	1.476633	1.694263
1	1.115739	2.913153	0.658580
8	-0.939763	2.276108	-0.807330
7	-0.865529	0.152026	0.206231
1	0.031672	-0.462608	0.317424
6	-1.886368	-0.375000	-0.743143
6	-3.115065	-0.743863	0.079619
1	-2.141180	0.400072	-1.471758
1	-1.488208	-1.245335	-1.270151
8	-3.169966	-0.534962	1.275481
8	-4.065538	-1.291068	-0.666607
1	-4.841714	-1.505319	-0.110362
1	4.853521	-2.287688	-0.425262
1	-1.330056	0.150548	1.141259

Figure 8. Structure TS(XI-product), B3LYP/6-31+G(d)

Electronic energy =-700.1843705 hartree

7	-4.204754	-0.850163	-0.660530
1	-3.800266	-1.697024	-0.276061
6	-3.542012	0.320251	-0.592492
6	-2.235212	0.374482	-0.071641
1	-4.038364	1.212931	-0.953523
8	-1.623084	-0.700261	0.344787
7	-1.493144	1.506208	0.032719
1	-1.897805	2.425269	-0.098834
6	-0.302607	1.313210	0.850646
6	-0.121937	-0.202945	0.938662
1	0.577429	1.784847	0.407685
1	-0.448655	1.684302	1.872826
8	0.329857	-0.854472	1.826750
7	0.748510	-0.708487	-0.678870

1	0.187638	-1.494465	-1.007679
6	2.136165	-1.124635	-0.406824
6	3.037234	0.096716	-0.433417
1	2.168608	-1.593598	0.583778
1	2.489927	-1.858199	-1.139698
8	2.635308	1.217246	-0.681733
8	4.302395	-0.223103	-0.162871
1	4.854698	0.583384	-0.194642
1	-5.159878	-0.893226	-0.990543
1	0.726797	0.035120	-1.381606