Supporting Information

Photoinduced Water Oxidation at the Aqueous GaN $(10\bar{1}0)$ Interface: Deprotonation Kinetics of the First Proton-Coupled Electron-Transfer Step

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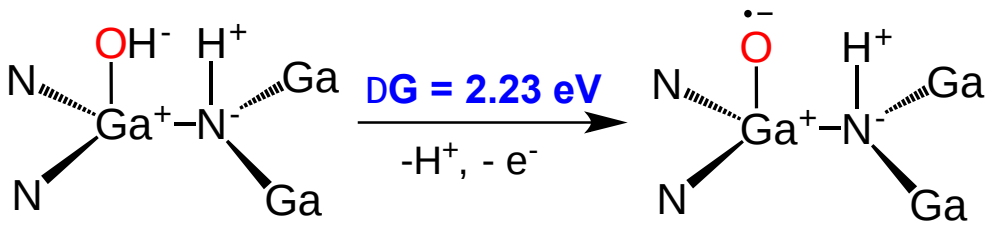
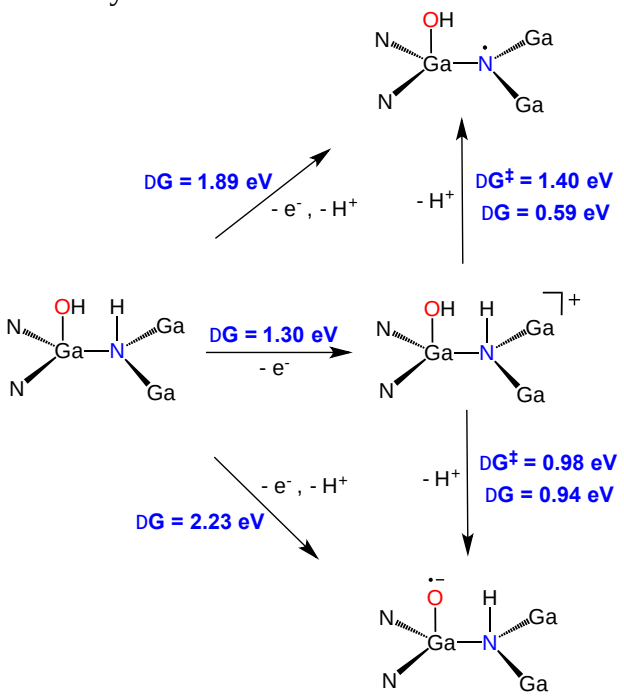
Bonding in tetrahedral Wurtzite GaN. The bonding in bulk Wurtzite GaN is best described as follows. Each group III Ga atom (s^2p) accepts an electron from a group V N atom (s^2p^3) so that both the resulting Ga^- and N^+ species take on group IV (s^2p^2), carbon-like character. These Ga^- and N^+ species then form sp^3 hybrid orbitals which make a tetrahedral network of covalent bonds in which each Ga^- ion is bonded to four N^+ ions, and each N^+ ion is bonded to four Ga^- ions. The electron pair in each of these covalent bonds is polarized toward the N^+ ion to compensate for the initial charge transfer. This motif describes the Wurtzite structure of bulk GaN, but not the non-polar (10-10) surface. At the surface, there is a dangling bond (singly occupied sp^3 orbital) on every surface atom exposed to either vacuum or an aqueous interface. This is not a stable configuration, so the surface reconstructs by the transfer of the electrons in Ga dangling bonds to the corresponding dangling bonds on N atoms, resulting in an overall neutral surface composed of an equal number of Ga^+ and N^- ions. The vacant orbital on the Ga^+ ions give it Lewis acid properties, and the doubly occupied (lone pair) on the N^- ions imparts both Lewis and Brønsted base properties to them. The dissociation of a water molecule to OH^- and H^+ with essentially no energy barrier (reported as 1 meV in Shen, X.; Allen, P. B.; Hybertsen, M. S.; Muckerman, J. T. *J. Phys. Chem. C* **2009**, *113*, 3365-3368) is consistent with the long-range stabilization of the stretching of the H—OH bond imparted by the ionic character of the surface. A lone pair on the dissociated OH^- ion occupies the vacant orbital on a Ga^+ site, and the H^+ attaches to the lone pair of a N^- site.



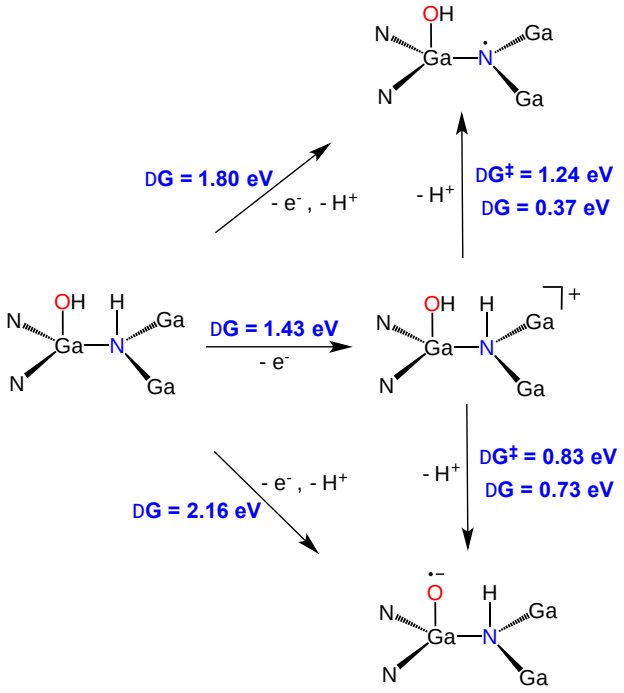
Molecular Cluster Model. The GaN $(10\bar{1}0)$ surface model was built from a representative structure obtained from ab initio molecular dynamics simulations, as detailed in the main text. The 3×2 GaN $(10\bar{1}0)$ surface model contains 28 Ga and 28 N atoms, twelve of which form –Ga-OH and –NH surface species upon the dissociation of 6 H_2O molecules. In addition to that, 7 H_2O molecules are included in the model to preserve the H-bonding interactions and first-shell solvation effects. The dangling bonds formed at terminal positions of the model were passivated with H atoms to complete the coordination number of Ga and N atoms. The two previous cluster models in Ref. 16 contain either (i) 15 Ga and 15 N atoms with 2 dissociated H_2O molecules and 4 additional explicit H_2O molecules or (ii) 21 Ga and 21 N atoms with 3 dissociated H_2O molecules and 4 additional explicit H_2O molecules. The present model is not only larger than previous models but details of the passivation of dangling bonds on Ga and N in the "interior" of the GaN semiconductor by hydrogen atoms have been improved. In the previous models, the presence of the polarizable continuum solvation model was essential to prevent (through stabilization of charge separation) a hydridic Ga–H hydrogen from reacting with a nearby acidic N–H hydrogen in certain regions where they were close enough to interact. In the present model, additional "bulk" GaN was added to an initial version of the present model to avoid such close interactions. Furthermore, the present model provides improvements in treating the hydrogen bonding interactions between

dissociated water molecules and first shell water molecules resulting in more compatible structures with AIMD simulations (*e.g.*, no strong H-bonding interactions with –NH sites).

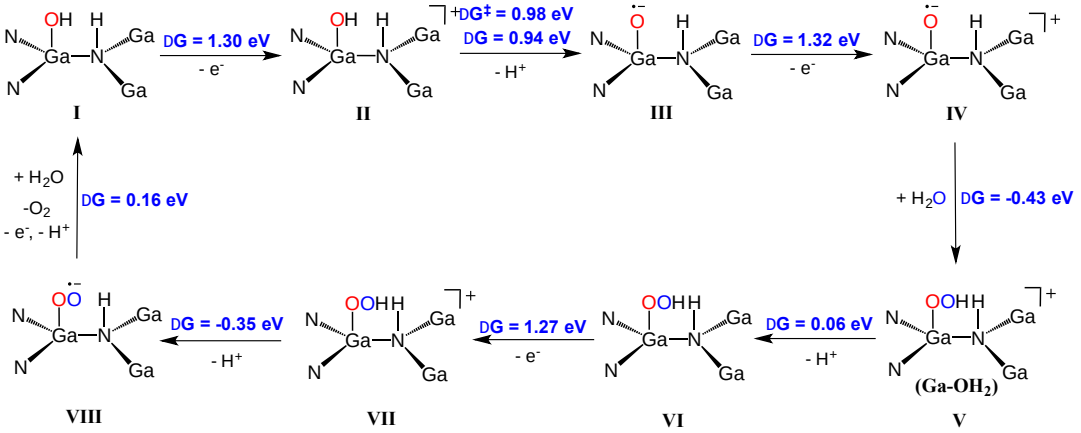
Scheme S1. Energetics of proton-coupled electron-transfer from –NH and –Ga-OH sites at the M11-L level of theory This scheme, which is the same as Scheme 1 in the main text, is repeated here for ready reference.



Scheme S2. Energetics of proton-coupled electron-transfer from –NH and –Ga-OH sites obtained via B3LYP single-point calculations on M11-L optimized structures.



Scheme S3. Proposed water oxidation mechanism at pH 4.0 using molecular cluster models. (Ga-OH_2) refers to protonation of a neighboring –Ga-OH site. This scheme, which is the same as Scheme 2 in the main text, is repeated here for ready reference.



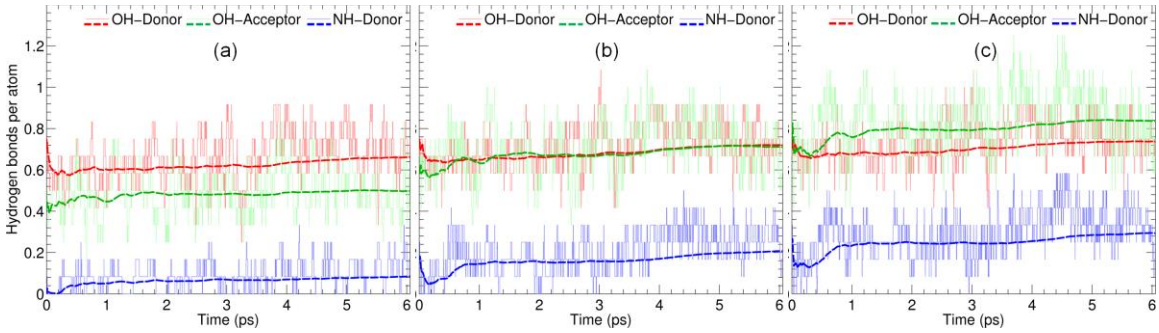


Figure S1. Time dependence of the number of hydrogen bonds between the hydroxylated GaN surface and the bulk water layer from the equilibrated portion of the MD simulation. The data in (a), (b) and (c) are obtained using the donor-acceptor distance cutoff of 3.0 Å, 3.25 Å, and 3.5 Å, respectively. Panel (a) is the same as Figure 2 in the main text. Instantaneous and time-averaged traces are depicted by thin continuous and thick dashed lines, respectively.

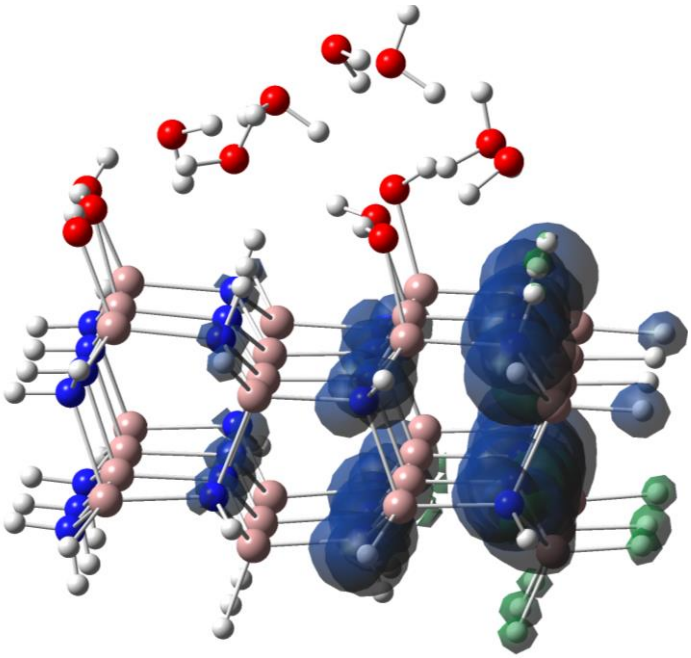


Figure S2. Unpaired spin density plot for **II** (doublet) in Scheme S3.

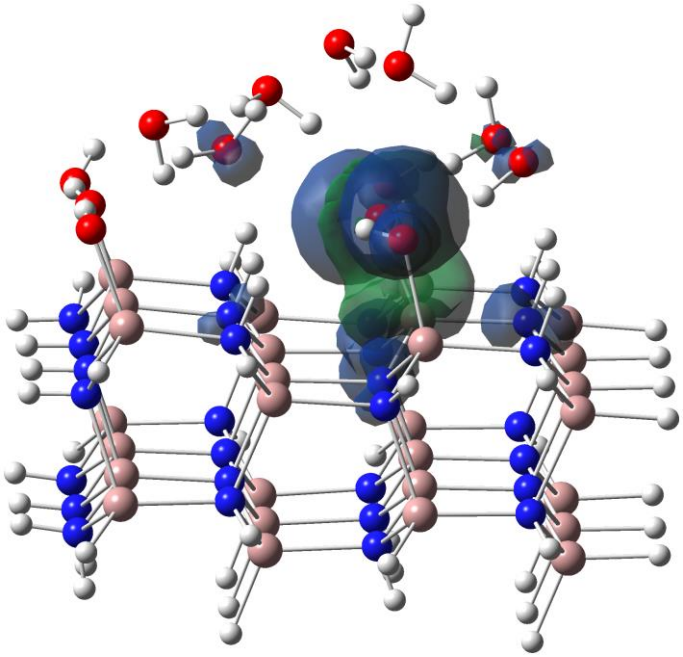


Figure S3. Unpaired spin density plot for **III** (doublet) in Scheme S3

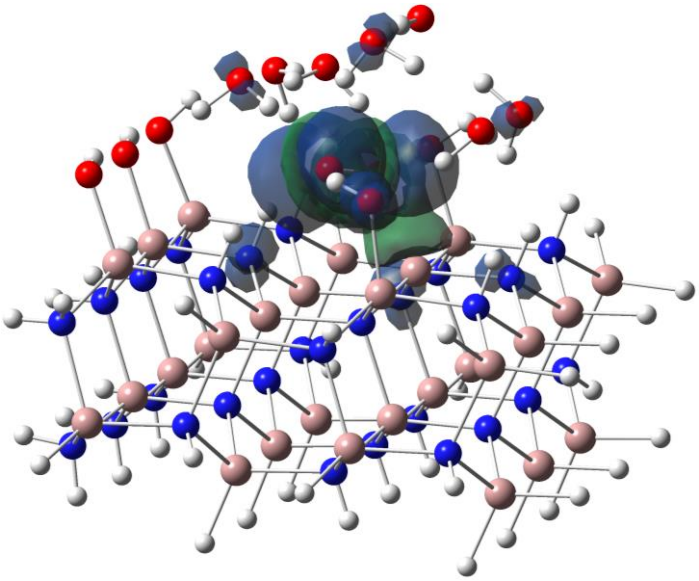


Figure S4. Unpaired spin density plot for **VIII** (doublet) in Scheme S3.

Table S1. Comparison of different density functionals for free-energy changes of PCET steps of proposed water oxidation mechanism at the aqueous GaN $(10\bar{1}0)$ interface via cluster models. Associated free-energy changes (ΔG*') in units of eV from cluster model calculations are reported at pH 4.0.(see computational methods for details).

	ΔG*' (eV vs NHE)	
	M11-L	**B3LYP**
–Ga-OH → –Ga-O$^{\bullet-}$ + H$^+$ + e^-	2.23	2.16
–Ga-O$^{\bullet-}$ + H_2O → –Ga-OOH + H$^+$ + e^-	0.96	0.83
–Ga-OOH → –Ga-OO$^{\bullet-}$ + H$^+$ + e^-	0.91	0.78
–Ga-OO$^{\bullet-}$ + H_2O → –Ga-OH + O_2 + H$^+$ + e^-	0.16	0.01

Table S2. Comparison of computed free-energy changes of PCET steps of proposed water oxidation mechanism at the aqueous GaN $(10\bar{1}0)$ interface at the B3LYP level of theory via cluster models of the present work and by Shen et al. (Ref 16). Associated free-energy changes (ΔG*') in units of eV from cluster model calculations are reported at pH 4.0.(see computational methods for details).

	ΔG*' (eV vs NHE)	
	This work (SDD/6-311G(d,p)	**Ref 16 SBKJC/6-311G(d,p)**
–Ga-OH → –Ga-O$^{\bullet-}$ + H$^+$ + e^-	2.18	2.32
–Ga-O$^{\bullet-}$ + H_2O → –Ga-OOH + H$^+$ + e^-	0.60	0.75
–Ga-OOH → –Ga-OO$^{\bullet-}$ + H$^+$ + e^-	0.87	0.77
–Ga-OO$^{\bullet-}$ + H_2O → –Ga-OH + O_2 + H$^+$ + e^-	-0.20	-0.35

Geometry (Atomic Numbers Followed by the Cartesian Coordinates in Å) and Energy of Optimized Structures from Cluster Models

I (restricted singlet) in Scheme S3

E = -2611.28912555 a.u.

1	-3.486452	-1.149199	2.070792
1	-0.588025	-0.028948	3.320027
1	-0.284003	-1.649689	2.140460
1	-1.300474	-1.598973	4.782576
1	-1.251875	-2.791926	3.775718
1	1.315374	-5.107707	3.233345
1	-4.589929	-3.829066	3.202963
1	2.893775	-2.122888	2.376269
1	-1.825453	-4.637696	3.026957
1	-6.202903	-2.195911	2.528629
1	-5.416023	-1.862086	3.778168
1	-2.600984	1.800215	3.771582
1	-3.874739	-0.086709	4.074568
1	-3.357499	-1.469168	4.373266
1	1.269845	0.721360	7.306908
1	1.600102	1.264077	5.931258
1	2.121302	0.101999	3.461049
1	-0.482881	1.885120	4.184242
1	-0.810319	2.442208	5.563640
1	1.312628	2.835547	4.582961
1	2.510755	1.935342	4.261343
1	-0.457488	0.112964	6.084534
1	-1.812763	0.328568	5.427336
1	3.775570	3.113349	2.737608
1	-2.616886	4.113448	2.512119
1	0.563022	3.584723	2.602146
1	-3.810323	6.528883	0.754314
1	6.402174	2.978283	-1.316077
1	6.796244	2.520694	1.832483
1	2.549266	5.500065	1.019454
1	-0.592920	5.999990	0.910700
1	-5.361046	1.976352	0.873136
1	-6.495664	-0.786711	0.924500
1	-5.668674	-0.445712	-2.153402
1	-5.917370	2.101165	-2.288921
1	-5.542092	-4.733136	-0.179031
1	0.823771	-5.661419	0.175683
1	5.791766	-5.305939	-2.083746
1	4.936041	-5.259151	1.041362

1	5.955032	-2.785272	1.529132
1	5.777006	0.203973	1.353289
1	6.591761	0.034805	-1.746933
1	5.555261	-2.305084	-1.618953
1	-3.281337	-0.887032	-4.189036
1	-2.838674	1.909836	-3.222965
1	0.035195	-1.444620	-4.060277
1	0.417586	1.378876	-3.116931
1	3.364132	-2.022040	-3.875683
1	3.718873	0.808800	-2.963646
1	-6.796104	-3.205165	-2.767485
1	-6.277717	-3.436985	0.442423
1	-2.419027	-5.144429	-0.027924
1	-5.584597	4.504774	1.400329
1	5.799353	4.989760	1.078751
1	-4.840265	4.829030	-1.719140
1	3.873675	-6.267743	0.357918
1	4.129075	3.297066	-3.476257
1	4.391306	5.383132	-1.690285
1	0.835150	3.807726	-3.619589
1	1.111042	5.906324	-1.861865
1	-2.437590	4.383715	-3.711588
1	-2.147334	6.451775	-1.907945
1	-3.936858	-4.804765	-2.662625
1	-3.708067	-3.575475	-3.690759
1	-0.398810	-4.060660	-3.549802
1	-0.668594	-5.318433	-2.560488
1	2.860163	-4.675715	-3.331241
1	2.573356	-5.891819	-2.301488
7	-4.946001	-0.986857	-1.669210
7	-5.441390	-3.722982	-0.069206
7	1.499161	-1.983046	-1.474527
7	4.655735	-2.566806	-1.204217
7	2.930573	-2.442544	1.403364
7	-2.265838	-4.138393	0.079480
7	-1.755509	-1.448205	-1.622637
7	-3.521977	-1.427566	1.085768
7	-0.273267	-1.921385	1.153704
7	0.964223	-4.652266	0.272397
7	4.096915	-5.276577	0.460020
7	-4.590718	1.523063	0.374169
7	-4.110572	4.307153	-1.227831
7	0.321025	0.953937	-2.189788
7	3.587935	0.400836	-2.033697
7	4.944487	-0.005351	0.795485
7	-0.913182	3.816488	-1.181303

7	-2.649020	3.870777	1.518271
7	2.330030	3.295060	-1.066300
7	-2.940380	1.482328	-2.297954
7	-1.437817	1.044691	0.498254
7	1.799315	0.538654	0.597485
7	0.567027	3.303732	1.618120
7	5.510364	2.737928	-0.876797
7	3.807530	2.849106	1.749501
7	-3.792715	-3.794472	-2.697485
7	-0.498641	-4.311913	-2.565422
7	2.769773	-4.890535	-2.337545
8	-4.120526	-0.899411	4.557397
8	-1.580413	-1.884830	3.897734
8	2.270386	-5.153508	3.097560
8	-3.868246	-4.256470	2.718649
8	-0.873682	-4.477152	2.939252
8	-6.086675	-2.484697	3.439875
8	-3.217965	1.308120	3.213855
8	0.154563	0.586293	3.263607
8	1.286021	0.462071	6.380822
8	3.056634	0.357424	3.464017
8	-0.803386	2.696118	4.634523
8	2.220636	2.651821	4.858291
8	-1.374574	-0.216228	6.089156
31	-5.071897	-0.409671	0.267591
31	-5.475886	-2.870780	-1.942221
31	-3.212763	-0.476322	-2.627942
31	0.031242	-1.011734	-2.499833
31	3.274764	-1.557159	-2.330304
31	4.798254	-1.994997	0.736636
31	-3.809764	-3.374913	1.068654
31	-1.755951	-0.885340	0.283119
31	1.517465	-1.395683	0.421896
31	-2.085140	-3.351976	-1.744405
31	1.214771	-3.895990	-1.557540
31	-0.619578	-3.871404	1.169033
31	4.575397	-4.531753	-1.407037
31	2.579515	-4.374801	1.420818
31	-4.555279	2.385767	-1.469674
31	-4.179526	4.944862	0.699789
31	2.035663	1.368605	-1.212858
31	5.327797	0.767634	-1.056311
31	-0.881650	4.414124	0.711317
31	-1.240659	1.896456	-1.326946
31	-2.951494	1.925420	1.420564
31	0.241646	1.357629	1.501096

31	3.422360	0.917147	1.673113
31	2.351342	3.899343	0.827730
31	5.647514	3.368963	1.046623
31	4.091461	3.790599	-1.915379
31	0.862060	4.294013	-2.052381
31	-2.357455	4.846569	-2.143614

II (doublet) in Scheme S3

E = -2611.08759176 a.u.

1	-3.505243	-1.106828	2.066917
1	-0.578111	-0.063359	3.344170
1	-0.308568	-1.672809	2.143778
1	-1.314152	-1.613457	4.792000
1	-1.277437	-2.802494	3.780521
1	1.265904	-5.137218	3.224969
1	-4.632394	-3.775150	3.199102
1	2.871683	-2.171317	2.376555
1	-1.906489	-4.616994	3.012175
1	-6.227821	-2.118826	2.523304
1	-5.435066	-1.805562	3.774480
1	-2.578014	1.821014	3.777471
1	-3.867134	-0.057715	4.078321
1	-3.365119	-1.448363	4.366813
1	1.267215	0.667459	7.327292
1	1.611283	1.222285	5.960074
1	2.123480	0.059041	3.486191
1	-0.463656	1.863986	4.201531
1	-0.803355	2.439797	5.569808
1	1.330578	2.798017	4.623012
1	2.522459	1.893350	4.290915
1	-0.463075	0.098368	6.093166
1	-1.811073	0.323833	5.423576
1	3.775893	3.068715	2.760180
1	-2.533988	4.132531	2.533147
1	0.593870	3.542047	2.641709
1	-3.671080	6.598262	0.765008
1	6.361955	2.972138	-1.317309
1	6.767157	2.457263	1.829340
1	2.583815	5.476297	1.022044
1	-0.485909	6.003113	0.910528
1	-5.322885	2.069613	0.860487
1	-6.503074	-0.676068	0.926358
1	-5.665946	-0.358916	-2.159631

1	-5.850066	2.243245	-2.310952
1	-5.610615	-4.655383	-0.190729
1	0.764937	-5.681759	0.166270
1	5.741214	-5.346046	-2.101591
1	4.878690	-5.318942	1.024276
1	5.934991	-2.825414	1.526780
1	5.767916	0.159298	1.352615
1	6.588118	0.029706	-1.750749
1	5.525999	-2.352022	-1.625131
1	-3.283145	-0.828807	-4.195772
1	-2.781690	1.946757	-3.223626
1	0.020854	-1.454926	-4.067645
1	0.440016	1.363211	-3.113323
1	3.334932	-2.035854	-3.883895
1	3.705339	0.783154	-2.958974
1	-6.842772	-3.093369	-2.772825
1	-6.327001	-3.350186	0.434848
1	-2.501559	-5.115100	-0.036659
1	-5.470665	4.577752	1.393727
1	5.815784	4.960593	1.096007
1	-4.679393	4.927934	-1.717219
1	3.807381	-6.311193	0.331669
1	4.093871	3.260272	-3.476948
1	4.370809	5.368661	-1.679642
1	0.881450	3.744186	-3.636634
1	1.187447	5.893233	-1.905466
1	-2.293889	4.409118	-3.711219
1	-1.971954	6.488411	-1.887262
1	-4.012207	-4.744640	-2.681831
1	-3.760153	-3.512468	-3.700855
1	-0.448219	-4.051174	-3.559847
1	-0.732966	-5.311087	-2.578372
1	2.809249	-4.695338	-3.344106
1	2.519759	-5.916988	-2.321869
7	-4.953623	-0.911376	-1.672456
7	-5.494640	-3.647189	-0.077163
7	1.475354	-2.007405	-1.474715
7	4.625062	-2.606213	-1.208416
7	2.907812	-2.484385	1.401403
7	-2.325761	-4.112351	0.069196
7	-1.772660	-1.433362	-1.626955
7	-3.545107	-1.380325	1.080650
7	-0.298649	-1.939052	1.155476
7	0.909742	-4.673111	0.263751
7	4.040213	-5.322979	0.441612
7	-4.561287	1.599646	0.362985

7	-3.984163	4.371311	-1.211063
7	0.334804	0.933473	-2.189253
7	3.583826	0.369248	-2.030132
7	4.935440	-0.047142	0.793057
7	-0.830013	3.795984	-1.145288
7	-2.578795	3.892354	1.538734
7	2.328892	3.248631	-1.027887
7	-2.903176	1.522494	-2.299295
7	-1.426210	1.044680	0.504339
7	1.796871	0.500041	0.608913
7	0.599784	3.267741	1.654876
7	5.485107	2.707512	-0.858512
7	3.815430	2.799612	1.773021
7	-3.848077	-3.737038	-2.709012
7	-0.551920	-4.306341	-2.576710
7	2.718724	-4.915900	-2.351558
8	-4.120427	-0.870309	4.556374
8	-1.587449	-1.889002	3.901719
8	2.220110	-5.188962	3.087182
8	-3.914959	-4.205129	2.710862
8	-0.947877	-4.500463	2.923910
8	-6.115964	-2.414899	3.432658
8	-3.200779	1.337659	3.218168
8	0.161175	0.555641	3.281545
8	1.285413	0.418919	6.398275
8	3.059228	0.313300	3.480519
8	-0.769072	2.686932	4.639369
8	2.241102	2.611787	4.888861
8	-1.383707	-0.220675	6.092718
31	-5.076125	-0.333934	0.262045
31	-5.516981	-2.789660	-1.946980
31	-3.214010	-0.441570	-2.631830
31	0.017717	-1.036073	-2.507550
31	3.251591	-1.597284	-2.333932
31	4.775726	-2.044828	0.732885
31	-3.860329	-3.327247	1.060485
31	-1.768997	-0.888911	0.283446
31	1.496046	-1.438426	0.427204
31	-2.132944	-3.337739	-1.755834
31	1.166824	-3.922294	-1.567257
31	-0.673004	-3.889865	1.161106
31	4.527598	-4.574034	-1.419701
31	2.532162	-4.416115	1.410192
31	-4.492006	2.464547	-1.472400
31	-4.061398	5.026468	0.706587
31	2.034904	1.317067	-1.195064

31	5.316961	0.732020	-1.049508
31	-0.806806	4.430316	0.738734
31	-1.205112	1.878958	-1.313980
31	-2.927383	1.948171	1.431090
31	0.245864	1.319231	1.525673
31	3.419306	0.861836	1.692569
31	2.375061	3.884386	0.855207
31	5.642131	3.349548	1.054159
31	4.098894	3.789413	-1.941112
31	0.919805	4.303954	-2.113066
31	-2.239475	4.912220	-2.168186

II-TS (doublet) in Scheme S3

E = -2611.04947898 a.u.

1	-3.363742	-1.375446	2.091345
1	-0.054076	-0.739764	3.691610
1	-0.140762	-1.610483	2.072378
1	0.177105	-1.662766	5.007289
1	-0.537759	-3.342058	3.523297
1	2.350941	-4.476235	3.649885
1	-3.989039	-3.994163	3.359386
1	3.034437	-1.885810	2.304427
1	-1.736235	-4.286001	3.120106
1	-5.524058	-2.320281	3.072188
1	-4.416302	-2.083200	4.083036
1	-2.743747	1.631096	3.759352
1	-2.969799	-0.391068	3.955837
1	-1.947445	-1.501295	4.294650
1	1.449998	0.000773	7.147840
1	1.399117	0.805984	5.865974
1	1.994455	0.237578	3.375546
1	-0.655609	1.626381	4.096587
1	-1.316655	1.871384	5.442596
1	0.950008	2.570763	4.778732
1	2.261088	1.918137	4.338481
1	-0.665690	0.137113	6.430966
1	-2.062845	-0.168851	5.907511
1	3.486462	3.303850	2.762867
1	-2.875866	3.915624	2.535837
1	0.315106	3.540343	2.644351
1	-4.222147	6.293795	0.768024
1	6.062442	3.469677	-1.322023
1	6.536329	2.978565	1.813911

1	2.143035	5.628446	1.036279
1	-0.955477	5.934895	0.930904
1	-5.491212	1.641422	0.893482
1	-6.393894	-1.225861	1.062641
1	-5.671480	-0.824908	-2.092264
1	-6.060130	1.766293	-2.283451
1	-5.224256	-5.095957	-0.092470
1	1.183568	-5.596288	0.204777
1	6.113331	-4.859083	-2.203280
1	5.285248	-4.921308	0.935867
1	6.129230	-2.386528	1.436503
1	5.734387	0.606825	1.294663
1	6.510806	0.569943	-1.824644
1	5.657551	-1.898446	-1.713708
1	-3.314163	-1.093218	-4.181600
1	-2.977123	1.719782	-3.213652
1	0.067182	-1.438370	-4.104045
1	0.265216	1.396254	-3.128556
1	3.438136	-1.746582	-3.952261
1	3.580197	1.083991	-3.000336
1	-6.630236	-3.669065	-2.647455
1	-6.017408	-3.837858	0.541737
1	-2.053906	-5.298501	-0.013303
1	-5.831519	4.127818	1.420461
1	5.343029	5.382482	1.102681
1	-5.103100	4.541477	-1.704233
1	4.279380	-5.980768	0.247653
1	3.781118	3.616169	-3.485551
1	3.903807	5.711049	-1.658387
1	0.529630	3.826703	-3.635401
1	0.682097	5.981946	-1.895956
1	-2.687332	4.209603	-3.699374
1	-2.531456	6.311163	-1.883136
1	-3.674024	-5.062153	-2.655660
1	-3.547818	-3.803895	-3.666762
1	-0.158911	-4.094029	-3.570101
1	-0.357946	-5.371984	-2.589884
1	3.104205	-4.496693	-3.380739
1	2.951730	-5.721473	-2.332665
7	-4.905225	-1.311186	-1.616277
7	-5.177989	-4.081547	0.013764
7	1.591667	-1.902650	-1.533062
7	4.786468	-2.226089	-1.285040
7	3.087625	-2.230031	1.339861
7	-1.974717	-4.282707	0.081555
7	-1.699047	-1.573994	-1.645349

7	-3.408518	-1.650993	1.105280
7	-0.151137	-1.912669	1.096818
7	1.273188	-4.579810	0.285988
7	4.442978	-4.979211	0.361385
7	-4.704659	1.228827	0.384046
7	-4.364916	4.041464	-1.199901
7	0.206429	0.956897	-2.204728
7	3.492809	0.656130	-2.073773
7	4.916704	0.331975	0.743239
7	-1.166938	3.728599	-1.139699
7	-2.901481	3.681921	1.539148
7	2.026877	3.430273	-1.041817
7	-3.060795	1.286148	-2.289389
7	-1.526814	0.936639	0.495423
7	1.740254	0.634901	0.556742
7	0.317651	3.272282	1.654109
7	5.206957	3.133660	-0.869734
7	3.555876	3.049135	1.773120
7	-3.592544	-4.044490	-2.675494
7	-0.249171	-4.356901	-2.587394
7	3.059348	-4.707338	-2.382747
8	-2.856132	-1.200955	4.496809
8	-0.192243	-1.752650	4.121560
8	2.868765	-5.026886	3.054432
8	-3.390198	-4.467583	2.761140
8	-0.748883	-4.185777	3.051270
8	-5.226754	-2.603009	3.943572
8	-3.368923	1.123618	3.218950
8	0.118600	0.482426	3.235756
8	1.165080	-0.063171	6.231089
8	2.960316	0.393061	3.392031
8	-1.068579	2.355148	4.636157
8	1.881757	2.487405	5.030054
8	-1.600319	0.365435	6.571846
31	-5.048575	-0.740532	0.319640
31	-5.313117	-3.232668	-1.868449
31	-3.229592	-0.694389	-2.621870
31	0.046742	-1.030137	-2.542263
31	3.322924	-1.329438	-2.399058
31	4.920060	-1.667100	0.659642
31	-3.560080	-3.610508	1.092280
31	-1.716313	-0.993822	0.256432
31	1.607581	-1.300751	0.352699
31	-1.896855	-3.499761	-1.769465
31	1.448210	-3.835074	-1.594906
31	-0.345119	-3.846514	1.090945

31	4.852794	-4.193296	-1.496312
31	2.910070	-4.179555	1.389006
31	-4.718009	2.095228	-1.451733
31	-4.471825	4.692884	0.716098
31	1.874887	1.483127	-1.221408
31	5.195860	1.158680	-1.097508
31	-1.165585	4.341883	0.751065
31	-1.386589	1.788939	-1.304227
31	-3.086011	1.714953	1.430894
31	0.134607	1.272390	1.574818
31	3.324206	1.089580	1.662225
31	2.033873	4.025306	0.856151
31	5.326773	3.762874	1.053230
31	3.746914	4.119213	-1.940226
31	0.538089	4.375327	-2.105261
31	-2.664735	4.715159	-2.154717

III (doublet) in Scheme S3

E = -2610.59972887 a.u.

1	-3.504441	-1.145273	2.063700
1	-0.317144	-1.633363	2.163978
1	-1.369116	-1.669819	4.739116
1	-1.310788	-2.916624	3.802465
1	1.282043	-5.118419	3.223352
1	-4.631528	-3.844308	3.159391
1	2.886869	-2.154143	2.387860
1	-1.867274	-4.700983	2.977598
1	-6.253840	-2.190966	2.475494
1	-5.478141	-1.871476	3.735238
1	-2.670004	1.798440	3.792481
1	-3.915596	-0.113655	4.062253
1	-3.451255	-1.513995	4.379395
1	1.254184	0.452283	7.217046
1	1.539372	1.137296	5.894786
1	2.255366	-0.171995	3.447746
1	-0.591354	1.831533	4.181777
1	-0.904687	2.381195	5.562392
1	1.201513	2.750859	4.606968
1	2.399285	1.858462	4.247057
1	-0.519371	0.028254	6.012803
1	-1.881792	0.251032	5.367628
1	3.787183	3.076571	2.772376
1	-2.592960	4.116197	2.538580

1	0.588922	3.574257	2.625974
1	-3.767154	6.546048	0.795446
1	6.428757	2.955361	-1.277041
1	6.809575	2.470467	1.868030
1	2.593515	5.488012	1.053903
1	-0.565413	6.006822	0.947703
1	-5.344364	2.006581	0.875947
1	-6.499824	-0.747505	0.911894
1	-5.661367	-0.391686	-2.164390
1	-5.892964	2.155645	-2.291025
1	-5.557978	-4.701748	-0.235902
1	0.789425	-5.656501	0.162132
1	5.765526	-5.326510	-2.089759
1	4.902636	-5.291726	1.033938
1	5.939664	-2.819147	1.539491
1	5.779554	0.170159	1.366908
1	6.605695	0.013237	-1.736400
1	5.546138	-2.327192	-1.610551
1	-3.265864	-0.843941	-4.189949
1	-2.816811	1.947096	-3.216319
1	0.044221	-1.426527	-4.051884
1	0.438013	1.393459	-3.108426
1	3.351049	-2.025509	-3.863777
1	3.736947	0.798702	-2.954408
1	-6.802951	-3.137623	-2.810971
1	-6.300309	-3.415774	0.397854
1	-2.439593	-5.121115	-0.056493
1	-5.557798	4.527732	1.420008
1	5.831226	4.952751	1.126690
1	-4.803142	4.871768	-1.693315
1	3.833411	-6.287772	0.343046
1	4.164734	3.293795	-3.445358
1	4.432794	5.371838	-1.649335
1	0.870172	3.829233	-3.590633
1	1.155052	5.914631	-1.815931
1	-2.401139	4.420763	-3.687254
1	-2.100745	6.479701	-1.873291
1	-3.953680	-4.757577	-2.695670
1	-3.710965	-3.526911	-3.718877
1	-0.406388	-4.020081	-3.567383
1	-0.689872	-5.287903	-2.595116
1	2.839569	-4.673026	-3.339732
1	2.542554	-5.890473	-2.314571
7	-4.945238	-0.942328	-1.681169
7	-5.460683	-3.692638	-0.113330
7	1.491749	-1.978563	-1.461804

7	4.644988	-2.585608	-1.197219
7	2.918549	-2.459891	1.410506
7	-2.286280	-4.115393	0.054620
7	-1.755121	-1.421935	-1.621311
7	-3.534526	-1.412439	1.075503
7	-0.288211	-1.916754	1.179116
7	0.937786	-4.648589	0.260556
7	4.064746	-5.299025	0.450600
7	-4.577525	1.551407	0.373249
7	-4.076827	4.342278	-1.205103
7	0.338331	0.969048	-2.181375
7	3.603397	0.393084	-2.023878
7	4.949582	-0.033246	0.803056
7	-0.884140	3.833125	-1.157100
7	-2.625119	3.876619	1.543986
7	2.359442	3.290967	-1.039856
7	-2.921743	1.517679	-2.292573
7	-1.425679	1.053866	0.506402
7	1.810226	0.530055	0.604444
7	0.590959	3.306669	1.638486
7	5.533846	2.715296	-0.843732
7	3.823740	2.821304	1.782035
7	-3.803067	-3.748045	-2.726794
7	-0.513528	-4.282484	-2.586680
7	2.746259	-4.890488	-2.346922
8	-4.195700	-0.914430	4.545373
8	-1.722922	-2.045983	3.918210
8	2.236777	-5.169715	3.087696
8	-3.912255	-4.270754	2.670881
8	-0.910046	-4.575917	2.891070
8	-6.140047	-2.495016	3.382077
8	-3.230129	1.276056	3.204325
8	0.083919	0.506531	3.221571
8	1.246142	0.290064	6.269081
8	3.065757	0.351463	3.476489
8	-0.863642	2.651186	4.638393
8	2.116710	2.567249	4.857989
8	-1.443568	-0.278706	6.041530
31	-5.072652	-0.377701	0.258883
31	-5.485695	-2.819291	-1.975203
31	-3.203704	-0.438600	-2.627087
31	0.035824	-0.995603	-2.490889
31	3.270973	-1.562701	-2.317255
31	4.789429	-2.022560	0.744534
31	-3.836034	-3.358639	1.038852
31	-1.758892	-0.877470	0.290626

31	1.506509	-1.404810	0.438166
31	-2.097884	-3.322472	-1.762412
31	1.195931	-3.889625	-1.564908
31	-0.645469	-3.866894	1.161072
31	4.552421	-4.548834	-1.411473
31	2.552536	-4.390795	1.412470
31	-4.533957	2.426310	-1.462599
31	-4.148896	4.965765	0.727190
31	2.057233	1.367951	-1.205564
31	5.344829	0.747234	-1.042695
31	-0.858762	4.424393	0.736970
31	-1.221629	1.917529	-1.322779
31	-2.941099	1.935153	1.431372
31	0.261091	1.369202	1.486114
31	3.433175	0.896242	1.677783
31	2.384202	3.890906	0.854884
31	5.670608	3.333587	1.085136
31	4.126308	3.782408	-1.883320
31	0.897589	4.306016	-2.021137
31	-2.320977	4.877719	-2.118027

IV (triplet) in Scheme S3

E = -2610.39760452 a.u.

1	-3.524920	-1.097895	2.059786
1	-0.342681	-1.652297	2.167485
1	-1.382562	-1.668467	4.741192
1	-1.346101	-2.914531	3.802960
1	1.232487	-5.160015	3.211737
1	-4.679477	-3.787374	3.158613
1	2.864881	-2.202666	2.387434
1	-1.949902	-4.675142	2.966882
1	-6.279240	-2.107994	2.473862
1	-5.498168	-1.811860	3.736098
1	-2.650380	1.819332	3.796287
1	-3.911377	-0.083572	4.067998
1	-3.458167	-1.489921	4.373525
1	1.263796	0.399606	7.237054
1	1.558567	1.095870	5.922957
1	2.252946	-0.222014	3.464766
1	-0.567287	1.816996	4.195488
1	-0.894164	2.392912	5.561499
1	1.227069	2.713558	4.648634
1	2.414554	1.813756	4.273581

1	-0.518657	0.018140	6.028799
1	-1.873507	0.259429	5.373891
1	3.787070	3.028916	2.795228
1	-2.510903	4.133896	2.559277
1	0.620850	3.529222	2.666918
1	-3.625895	6.616056	0.805802
1	6.387579	2.947569	-1.278567
1	6.783504	2.406658	1.862239
1	2.627747	5.461803	1.056139
1	-0.455873	6.008770	0.948640
1	-5.307030	2.101687	0.858453
1	-6.506655	-0.636224	0.913000
1	-5.659361	-0.304543	-2.172221
1	-5.819799	2.301409	-2.318219
1	-5.630433	-4.619886	-0.243189
1	0.724672	-5.675526	0.156159
1	5.712188	-5.368642	-2.109921
1	4.845593	-5.346649	1.016663
1	5.918383	-2.863070	1.534121
1	5.770978	0.122335	1.364846
1	6.602913	0.006555	-1.741199
1	5.514623	-2.375496	-1.618479
1	-3.268178	-0.786487	-4.197601
1	-2.756351	1.982677	-3.219982
1	0.026403	-1.438335	-4.059234
1	0.461877	1.374984	-3.106445
1	3.318296	-2.041742	-3.872955
1	3.723958	0.770438	-2.951171
1	-6.848600	-3.026386	-2.814930
1	-6.351716	-3.322203	0.391376
1	-2.523055	-5.090190	-0.059521
1	-5.443237	4.602724	1.410371
1	5.846193	4.921143	1.142343
1	-4.637513	4.972148	-1.692630
1	3.770739	-6.331532	0.319321
1	4.128932	3.252628	-3.446995
1	4.412839	5.354748	-1.641591
1	0.917816	3.765500	-3.608050
1	1.233430	5.901559	-1.859289
1	-2.251814	4.450199	-3.686373
1	-1.921625	6.517473	-1.847759
1	-4.029733	-4.698764	-2.712504
1	-3.762331	-3.465868	-3.726848
1	-0.460773	-4.024335	-3.572472
1	-0.758349	-5.286756	-2.598160
1	2.784891	-4.692485	-3.351498

1	2.486140	-5.916424	-2.334865
7	-4.953369	-0.865713	-1.685812
7	-5.515889	-3.612721	-0.118671
7	1.465793	-2.004396	-1.462128
7	4.612320	-2.626789	-1.202891
7	2.894821	-2.503056	1.408310
7	-2.348411	-4.087437	0.049056
7	-1.774396	-1.407685	-1.625382
7	-3.558360	-1.362656	1.070966
7	-0.314631	-1.930302	1.180873
7	0.880235	-4.668553	0.254904
7	4.008259	-5.344784	0.432291
7	-4.548360	1.629093	0.358883
7	-3.947187	4.407020	-1.189032
7	0.353662	0.946631	-2.182087
7	3.599760	0.358610	-2.021844
7	4.940599	-0.077419	0.799718
7	-0.798903	3.811971	-1.119906
7	-2.554730	3.898167	1.563721
7	2.358362	3.242025	-1.001321
7	-2.881080	1.557532	-2.296525
7	-1.414087	1.055329	0.511000
7	1.807772	0.490620	0.615113
7	0.624311	3.268742	1.676643
7	5.507790	2.682072	-0.825649
7	3.832050	2.769299	1.805734
7	-3.858647	-3.692203	-2.736248
7	-0.570275	-4.283315	-2.590986
7	2.692445	-4.916675	-2.359964
8	-4.195957	-0.884207	4.547576
8	-1.732500	-2.031381	3.912638
8	2.187047	-5.210605	3.076258
8	-3.965016	-4.217459	2.666347
8	-0.988398	-4.582978	2.881851
8	-6.171825	-2.420060	3.378381
8	-3.217286	1.306184	3.206390
8	0.091395	0.471853	3.240291
8	1.252393	0.249091	6.287192
8	3.062694	0.302787	3.489182
8	-0.815308	2.651896	4.636684
8	2.145764	2.526510	4.885330
8	-1.446889	-0.276735	6.050103
31	-5.076950	-0.300264	0.251514
31	-5.525836	-2.738040	-1.979075
31	-3.205585	-0.403908	-2.632175
31	0.019943	-1.021413	-2.498595

31	3.245291	-1.605126	-2.321847
31	4.765563	-2.074574	0.739304
31	-3.889338	-3.308163	1.034464
31	-1.773110	-0.878960	0.290416
31	1.484073	-1.447788	0.443242
31	-2.147324	-3.308792	-1.770088
31	1.145670	-3.916943	-1.572389
31	-0.700396	-3.880108	1.155784
31	4.502888	-4.592640	-1.425203
31	2.504092	-4.433218	1.402342
31	-4.465979	2.506108	-1.468621
31	-4.028504	5.048221	0.733507
31	2.057317	1.313706	-1.188633
31	5.334013	0.708552	-1.036924
31	-0.781902	4.439075	0.767092
31	-1.183616	1.899699	-1.310742
31	-2.918340	1.958665	1.439796
31	0.264618	1.330002	1.510139
31	3.430113	0.839068	1.695677
31	2.408239	3.872836	0.884319
31	5.665462	3.311544	1.092841
31	4.134003	3.778608	-1.910522
31	0.958175	4.316341	-2.081987
31	-2.198195	4.945949	-2.141570

V (restricted singlet) in Scheme S3

E = -2686.84566332 a.u.

1	-3.463127	-1.298915	2.064963
1	-0.266928	-1.637107	2.120424
1	-0.655409	-2.648826	5.489963
1	-0.747820	-3.879197	3.539203
1	1.560405	-5.160537	3.194590
1	-4.158867	-3.914162	3.255949
1	2.992129	-2.042306	2.325713
1	-1.959465	-4.614100	2.914044
1	-5.686927	-2.179560	2.947531
1	-4.645865	-1.951181	4.029113
1	-2.800410	1.771779	3.762085
1	-3.148945	-0.272269	3.956836
1	-2.367438	-1.557035	4.359277
1	1.943981	-0.190178	6.373090
1	1.609970	1.247255	5.987310
1	2.626684	-0.039204	3.523456

1	-0.689383	1.828422	4.086642
1	-1.228253	2.073268	5.459843
1	1.152835	2.677316	4.605863
1	2.469157	1.962408	4.238721
1	-0.719437	0.223954	6.341246
1	-2.134799	-0.030381	5.826111
1	3.731497	3.234076	2.671449
1	-2.757855	4.019914	2.516128
1	0.458913	3.575867	2.615289
1	-4.032359	6.417401	0.776214
1	6.267929	3.200726	-1.443153
1	6.731050	2.756154	1.717448
1	2.321873	5.580177	1.012135
1	-0.749251	5.964463	0.946467
1	-5.434082	1.809907	0.877377
1	-6.442002	-1.021441	1.007639
1	-5.693113	-0.597374	-2.137630
1	-6.019650	1.943044	-2.293269
1	-5.449059	-4.894098	-0.198298
1	0.974235	-5.637683	0.141493
1	5.917055	-5.118426	-2.193675
1	5.091810	-5.105433	0.943888
1	6.035970	-2.592851	1.439464
1	5.803998	0.382140	1.215405
1	6.535454	0.261976	-1.936239
1	5.585998	-2.123220	-1.722718
1	-3.312196	-0.966793	-4.197313
1	-2.939251	1.847518	-3.236580
1	0.053303	-1.422763	-4.076908
1	0.357506	1.405464	-3.114000
1	3.335421	-1.903435	-3.930095
1	3.586065	0.933728	-3.015349
1	-6.737444	-3.396672	-2.781556
1	-6.181133	-3.596863	0.430393
1	-2.259859	-5.217021	-0.113774
1	-5.728504	4.327279	1.430014
1	5.647088	5.189113	0.952962
1	-5.019727	4.702184	-1.699424
1	4.054193	-6.143745	0.268307
1	3.916054	3.433308	-3.533697
1	4.159418	5.522965	-1.744666
1	0.668224	3.833305	-3.622913
1	0.904900	5.941471	-1.868944
1	-2.600309	4.344465	-3.694901
1	-2.376081	6.404629	-1.869562
1	-3.827662	-4.894977	-2.723507

1	-3.658374	-3.648590	-3.742126
1	-0.283025	-4.043733	-3.617399
1	-0.543063	-5.315458	-2.643062
1	2.942521	-4.602977	-3.392830
1	2.711798	-5.813433	-2.342594
7	-4.951697	-1.123668	-1.665088
7	-5.352582	-3.883216	-0.093371
7	1.521528	-1.935371	-1.492131
7	4.704367	-2.418217	-1.292103
7	3.014499	-2.355516	1.349930
7	-2.145717	-4.206649	0.001754
7	-1.748072	-1.483126	-1.647019
7	-3.481359	-1.549594	1.071644
7	-0.241754	-1.938530	1.143675
7	1.089435	-4.625358	0.239638
7	4.247918	-5.146363	0.370419
7	-4.659075	1.382325	0.362688
7	-4.275248	4.195314	-1.214463
7	0.254983	0.974368	-2.190141
7	3.513362	0.518863	-2.081808
7	4.968006	0.155805	0.669129
7	-1.061184	3.800973	-1.172446
7	-2.778417	3.791452	1.518504
7	2.190466	3.363582	-1.078386
7	-3.024285	1.415863	-2.311919
7	-1.483886	1.008770	0.476573
7	1.789133	0.575743	0.622261
7	0.460745	3.294889	1.631004
7	5.400157	2.919331	-0.980929
7	3.740973	2.988197	1.677891
7	-3.718351	-3.879970	-2.749714
7	-0.395199	-4.305357	-2.636919
7	2.876809	-4.807115	-2.394866
8	-3.162543	-1.039311	4.568306
8	-0.794615	-2.516132	4.546618
8	2.510056	-5.099648	3.043565
8	-3.622199	-4.429000	2.633018
8	-0.966248	-4.576206	2.876148
8	-5.413240	-2.509573	3.810135
8	-3.374928	1.250040	3.186917
8	-0.349323	0.374616	3.104264
8	1.197905	0.407174	6.258760
8	3.398920	0.533421	3.444760
8	-0.916247	2.565030	4.680496
8	2.089065	2.625487	4.845826
8	-1.636728	0.500278	6.467540

31	-5.077935	-0.564738	0.277694
31	-5.424101	-3.018375	-1.966991
31	-3.243569	-0.546581	-2.639958
31	0.023373	-0.992250	-2.518021
31	3.271028	-1.447352	-2.382635
31	4.860697	-1.837528	0.641793
31	-3.718396	-3.496742	0.998252
31	-1.752722	-0.922429	0.262348
31	1.555306	-1.360224	0.404718
31	-2.013971	-3.389294	-1.827343
31	1.306737	-3.854535	-1.613885
31	-0.516061	-3.863702	1.044052
31	4.688016	-4.384606	-1.498305
31	2.723905	-4.295224	1.366354
31	-4.667226	2.263663	-1.472279
31	-4.349044	4.823014	0.716443
31	1.956708	1.433035	-1.218304
31	5.281510	0.946582	-1.183296
31	-1.027591	4.381624	0.725301
31	-1.337908	1.878405	-1.342462
31	-3.028239	1.841244	1.402348
31	0.201931	1.350910	1.472884
31	3.459917	1.044168	1.613089
31	2.218989	3.974384	0.812148
31	5.552740	3.565663	0.936387
31	3.914932	3.922097	-1.971706
31	0.689983	4.325525	-2.058476
31	-2.539138	4.797872	-2.124050
8	0.720670	-0.390379	3.679561
1	0.793916	0.000284	4.576154
1	-0.163567	-1.815143	4.302854

VI (restricted singlet) in Scheme S3

E = -2686.38903684 a.u.

1	-3.454622	-1.288269	2.058090
1	-0.257752	-1.653978	2.117641
1	-0.754163	-3.294401	3.903258
1	1.519985	-5.134951	3.145558
1	-4.256399	-3.873832	3.254333
1	2.989862	-2.036528	2.330230
1	-1.666240	-4.807419	2.920714
1	-5.726422	-2.095410	2.869291
1	-4.709176	-1.902478	3.981076

1	-2.833307	1.748571	3.747726
1	-3.158817	-0.307199	3.939533
1	-2.410525	-1.617243	4.340475
1	1.851994	-0.212449	6.401293
1	1.540373	1.223667	5.987766
1	2.581144	-0.018637	3.534301
1	-0.720693	1.834472	4.078810
1	-1.284519	2.075939	5.442203
1	1.113662	2.673635	4.617523
1	2.431263	1.957496	4.256595
1	-0.792790	0.250252	6.360969
1	-2.187314	-0.033227	5.807864
1	3.690284	3.247156	2.693467
1	-2.789432	4.004525	2.502399
1	0.425892	3.577915	2.614766
1	-4.075239	6.392968	0.756412
1	6.257573	3.240490	-1.402559
1	6.704101	2.796540	1.759524
1	2.290920	5.592306	1.021066
1	-0.788183	5.961449	0.936354
1	-5.444520	1.783177	0.854718
1	-6.443428	-1.041257	0.972780
1	-5.680512	-0.642208	-2.154679
1	-6.019840	1.908853	-2.320962
1	-5.405585	-4.916514	-0.168963
1	1.028788	-5.629985	0.104705
1	5.957727	-5.067624	-2.188769
1	5.132555	-5.058754	0.947089
1	6.046210	-2.559515	1.451357
1	5.792083	0.411311	1.245990
1	6.546420	0.307852	-1.899358
1	5.604057	-2.081974	-1.704967
1	-3.289673	-0.992782	-4.202941
1	-2.936238	1.819357	-3.250321
1	0.061698	-1.414076	-4.081879
1	0.362424	1.409278	-3.115421
1	3.368476	-1.865983	-3.925873
1	3.600569	0.966483	-2.998915
1	-6.706844	-3.449731	-2.760064
1	-6.148123	-3.621513	0.448702
1	-2.250378	-5.228259	-0.094253
1	-5.759109	4.292501	1.402112
1	5.603925	5.220147	0.993552
1	-5.038029	4.671731	-1.723926
1	4.115341	-6.119127	0.273288
1	3.922850	3.463036	-3.511988

1	4.135368	5.549722	-1.718164
1	0.666641	3.841209	-3.621676
1	0.879753	5.946320	-1.863177
1	-2.610156	4.326331	-3.709664
1	-2.404115	6.389053	-1.886958
1	-3.785086	-4.926832	-2.711868
1	-3.621727	-3.676195	-3.726453
1	-0.277325	-4.050172	-3.607982
1	-0.503739	-5.320277	-2.623770
1	2.992233	-4.557369	-3.404957
1	2.757403	-5.779251	-2.369152
7	-4.935348	-1.157445	-1.676384
7	-5.315772	-3.904319	-0.070920
7	1.539578	-1.917817	-1.498944
7	4.721711	-2.383769	-1.280706
7	3.022099	-2.344233	1.353019
7	-2.126866	-4.218868	0.019494
7	-1.731221	-1.496545	-1.645752
7	-3.471518	-1.553262	1.068889
7	-0.233278	-1.952508	1.139572
7	1.130710	-4.616639	0.206060
7	4.290002	-5.118197	0.373420
7	-4.665839	1.360119	0.342085
7	-4.292682	4.169515	-1.235450
7	0.259296	0.976819	-2.192352
7	3.523787	0.546569	-2.068063
7	4.960848	0.182718	0.693551
7	-1.077032	3.793557	-1.180223
7	-2.805133	3.775820	1.504761
7	2.177547	3.375671	-1.068915
7	-3.022344	1.391976	-2.323820
7	-1.487200	1.000934	0.467321
7	1.781015	0.581236	0.624688
7	0.434491	3.299379	1.629723
7	5.387957	2.953557	-0.947309
7	3.710550	3.003374	1.699496
7	-3.683672	-3.911101	-2.735112
7	-0.368815	-4.308465	-2.624658
7	2.917756	-4.771693	-2.409871
8	-3.188903	-1.069462	4.554227
8	-0.892486	-2.563795	4.533178
8	2.476720	-5.097576	3.021518
8	-3.641577	-4.374122	2.696882
8	-0.705744	-4.732793	2.798408
8	-5.505797	-2.414107	3.751372
8	-3.400742	1.226352	3.166228

8	-0.368864	0.387400	3.100912
8	1.115849	0.394127	6.272338
8	3.363564	0.541608	3.458671
8	-0.958595	2.570406	4.669841
8	2.045663	2.611304	4.870385
8	-1.715878	0.522968	6.448544
31	-5.066333	-0.591589	0.261221
31	-5.391429	-3.062239	-1.949551
31	-3.226591	-0.576492	-2.642867
31	0.034280	-0.993165	-2.518821
31	3.286810	-1.419668	-2.375143
31	4.862080	-1.812151	0.657251
31	-3.677962	-3.510317	1.036420
31	-1.738301	-0.939945	0.266488
31	1.549005	-1.362192	0.407590
31	-1.985574	-3.409142	-1.791339
31	1.332750	-3.838609	-1.615564
31	-0.488589	-3.916573	1.111296
31	4.716667	-4.349587	-1.495729
31	2.738639	-4.288565	1.351328
31	-4.671855	2.233832	-1.493173
31	-4.378357	4.795340	0.695371
31	1.953340	1.442182	-1.209385
31	5.280860	0.979700	-1.153470
31	-1.055448	4.375626	0.717523
31	-1.342404	1.866790	-1.347953
31	-3.039238	1.821985	1.386550
31	0.188798	1.351162	1.470182
31	3.438669	1.056161	1.628485
31	2.191784	3.985422	0.822409
31	5.522225	3.595559	0.972816
31	3.903506	3.946770	-1.948309
31	0.675952	4.328286	-2.055065
31	-2.556193	4.780036	-2.138074
8	0.690283	-0.393215	3.674698
1	0.727009	-0.041391	4.588824
1	-0.270742	-1.881478	4.239475

VII (doublet) in Scheme S3

E = -2686.18713534 a.u.

1	-3.473805	-1.263968	2.046468
1	-0.275787	-1.678991	2.124710
1	-0.826967	-3.316157	3.894645

1	1.491696	-5.172147	3.138209
1	-4.299242	-3.844030	3.237096
1	2.980373	-2.072548	2.336584
1	-1.722703	-4.820188	2.901994
1	-5.751220	-2.048722	2.845337
1	-4.742645	-1.865188	3.966981
1	-2.819537	1.769120	3.741642
1	-3.184182	-0.281400	3.940177
1	-2.452738	-1.594943	4.354794
1	1.636162	-0.208128	6.593076
1	1.442346	1.188972	5.997583
1	2.581773	-0.060324	3.549305
1	-0.715340	1.816011	4.118880
1	-1.347445	2.106619	5.443576
1	1.139871	2.662246	4.624892
1	2.441025	1.906403	4.295207
1	-0.922909	0.328964	6.432111
1	-2.295220	0.028707	5.837446
1	3.680674	3.217721	2.721695
1	-2.739322	4.020580	2.507850
1	0.443884	3.551400	2.652164
1	-3.967059	6.452609	0.740207
1	6.205307	3.254507	-1.396286
1	6.675199	2.760701	1.754617
1	2.310179	5.580456	1.028360
1	-0.710387	5.968074	0.941009
1	-5.415133	1.848396	0.822790
1	-6.451868	-0.958799	0.948759
1	-5.668725	-0.584949	-2.179158
1	-5.958750	2.023532	-2.361452
1	-5.461101	-4.861674	-0.191573
1	0.995638	-5.647910	0.102149
1	5.934016	-5.089112	-2.196445
1	5.102736	-5.097742	0.940305
1	6.037818	-2.579337	1.455241
1	5.787843	0.386250	1.249776
1	6.542323	0.329672	-1.897081
1	5.589796	-2.109199	-1.704484
1	-3.268137	-0.947797	-4.219999
1	-2.871495	1.847332	-3.256959
1	0.066019	-1.421204	-4.086450
1	0.387872	1.399658	-3.106630
1	3.351892	-1.867233	-3.927108
1	3.581307	0.954994	-2.985312
1	-6.727357	-3.371802	-2.790897
1	-6.182945	-3.553828	0.423595

1	-2.302136	-5.214450	-0.105440
1	-5.673278	4.352555	1.364386
1	5.600049	5.214243	1.014191
1	-4.894061	4.750262	-1.748468
1	4.081724	-6.149353	0.259151
1	3.875003	3.436415	-3.509905
1	4.090331	5.548982	-1.705276
1	0.709756	3.794873	-3.635503
1	0.944122	5.945433	-1.890998
1	-2.468155	4.330567	-3.720446
1	-2.249819	6.417341	-1.886419
1	-3.824678	-4.892712	-2.726766
1	-3.640405	-3.644849	-3.740883
1	-0.298209	-4.048050	-3.614040
1	-0.537639	-5.319222	-2.634683
1	2.965121	-4.568891	-3.408543
1	2.730654	-5.796076	-2.379244
7	-4.931218	-1.107229	-1.696323
7	-5.354031	-3.851081	-0.093688
7	1.528702	-1.935240	-1.491548
7	4.706649	-2.407034	-1.278824
7	3.010883	-2.375287	1.357630
7	-2.163750	-4.207015	0.009896
7	-1.735431	-1.488925	-1.650201
7	-3.490013	-1.525614	1.056121
7	-0.251588	-1.969624	1.144228
7	1.099931	-4.634810	0.205203
7	4.260509	-5.149681	0.365304
7	-4.639760	1.413326	0.314548
7	-4.182736	4.216302	-1.240009
7	0.274145	0.960083	-2.188094
7	3.517948	0.528481	-2.056275
7	4.955747	0.159173	0.697589
7	-1.002899	3.773357	-1.143282
7	-2.759286	3.792323	1.509673
7	2.166301	3.336028	-1.023861
7	-2.981368	1.420962	-2.332234
7	-1.474676	0.997245	0.475942
7	1.778103	0.551036	0.649240
7	0.454788	3.271256	1.666785
7	5.351308	2.942970	-0.923979
7	3.711715	2.969352	1.728502
7	-3.709428	-3.878338	-2.749585
7	-0.394754	-4.308405	-2.631665
7	2.891718	-4.788324	-2.414377
8	-3.227467	-1.038538	4.559419

8	-0.961521	-2.580258	4.519152
8	2.448568	-5.129821	3.018017
8	-3.687886	-4.348843	2.679732
8	-0.760410	-4.752599	2.789427
8	-5.538176	-2.373840	3.726864
8	-3.396698	1.256398	3.160429
8	-0.360671	0.360574	3.137252
8	0.958162	0.380938	6.247730
8	3.362931	0.502464	3.476962
8	-0.988965	2.571456	4.667243
8	2.055921	2.555204	4.914456
8	-1.850142	0.599722	6.483998
31	-5.066095	-0.541059	0.239044
31	-5.410526	-3.010584	-1.972898
31	-3.214904	-0.555770	-2.656577
31	0.033928	-1.015783	-2.523532
31	3.275553	-1.448048	-2.371826
31	4.850157	-1.843819	0.659320
31	-3.715435	-3.484414	1.021246
31	-1.744923	-0.949263	0.266387
31	1.535642	-1.396856	0.421195
31	-2.008496	-3.403433	-1.800926
31	1.307899	-3.860010	-1.616119
31	-0.522074	-3.936162	1.107190
31	4.692813	-4.376999	-1.499709
31	2.713719	-4.321232	1.349866
31	-4.615644	2.289450	-1.512365
31	-4.284768	4.864534	0.678236
31	1.948142	1.394656	-1.178209
31	5.267635	0.964539	-1.141108
31	-0.998525	4.392548	0.746097
31	-1.307842	1.846644	-1.332392
31	-3.022384	1.835464	1.386164
31	0.190856	1.315814	1.511157
31	3.439279	1.015392	1.654048
31	2.202445	3.980383	0.858779
31	5.505482	3.597076	0.986639
31	3.899299	3.959951	-1.973518
31	0.722882	4.352248	-2.111767
31	-2.452539	4.833679	-2.177171
8	0.694414	-0.453082	3.672108
1	0.736207	-0.127752	4.597957
1	-0.314260	-1.917484	4.237362

VIII (doublet) in Scheme S3

E = -2685.74714759 a.u.

1	-3.441691	-1.310843	2.079547
1	-0.266311	-1.728875	2.128174
1	-0.582936	-3.308296	3.933114
1	1.524854	-5.128074	3.152129
1	-4.229004	-3.894312	3.276337
1	2.985502	-2.039257	2.340322
1	-1.645648	-4.782005	2.951632
1	-5.654136	-2.066340	2.953691
1	-4.593127	-1.936595	4.034819
1	-3.218616	1.753651	3.809705
1	-2.981714	-0.423803	3.962473
1	-2.211850	-1.709180	4.400564
1	1.194965	-0.344256	5.372183
1	1.482551	1.030946	5.899713
1	2.888767	-0.112591	3.639826
1	-1.240150	2.800251	3.719204
1	-1.227939	2.180420	5.104824
1	0.942998	2.597126	4.575889
1	2.296206	1.930710	4.219478
1	-0.592467	0.462544	6.199235
1	-1.978918	0.046154	5.696009
1	3.664847	3.278373	2.675289
1	-2.818376	4.002747	2.537716
1	0.478040	3.620277	2.595635
1	-4.098393	6.362115	0.803516
1	6.240034	3.250570	-1.416696
1	6.684789	2.808924	1.744435
1	2.281970	5.620565	0.971856
1	-0.862204	5.976778	0.956308
1	-5.439017	1.761123	0.887439
1	-6.430770	-1.061129	1.023694
1	-5.690866	-0.656453	-2.119605
1	-6.034528	1.882892	-2.291191
1	-5.416406	-4.930662	-0.140687
1	1.055065	-5.642020	0.094893
1	5.959691	-5.054219	-2.186271
1	5.136216	-5.049421	0.950962
1	6.042730	-2.540679	1.458991
1	5.779327	0.427953	1.245309
1	6.537054	0.316184	-1.897741
1	5.598016	-2.069082	-1.699362
1	-3.308254	-0.999233	-4.180102
1	-2.945600	1.809414	-3.217828

1	0.051991	-1.416105	-4.068358
1	0.330979	1.408387	-3.100860
1	3.354648	-1.869475	-3.916870
1	3.592967	0.965847	-3.005894
1	-6.714788	-3.466051	-2.733411
1	-6.145280	-3.626888	0.475292
1	-2.259853	-5.248251	-0.100266
1	-5.784771	4.254050	1.433765
1	5.593280	5.236433	0.973655
1	-5.068946	4.651695	-1.688190
1	4.119334	-6.110556	0.277511
1	3.911789	3.451152	-3.538168
1	4.115402	5.553835	-1.759852
1	0.601021	3.841350	-3.619866
1	0.837701	5.944768	-1.857676
1	-2.647611	4.308320	-3.684527
1	-2.439095	6.375774	-1.865222
1	-3.788569	-4.931093	-2.711402
1	-3.634522	-3.670459	-3.714696
1	-0.276727	-4.033908	-3.604487
1	-0.497442	-5.314171	-2.632333
1	2.994106	-4.549861	-3.401487
1	2.758916	-5.770353	-2.364007
7	-4.943443	-1.173070	-1.646289
7	-5.317761	-3.918913	-0.047062
7	1.534060	-1.912122	-1.483494
7	4.717148	-2.374011	-1.274243
7	3.018794	-2.336783	1.360255
7	-2.129654	-4.240574	0.020987
7	-1.737740	-1.504079	-1.630265
7	-3.463666	-1.572297	1.089728
7	-0.238026	-1.981683	1.138723
7	1.139131	-4.627854	0.203613
7	4.293642	-5.109530	0.377433
7	-4.663657	1.340942	0.367410
7	-4.319440	4.151688	-1.203828
7	0.241326	0.974796	-2.176829
7	3.514949	0.550791	-2.073093
7	4.948798	0.197034	0.692596
7	-1.105761	3.785817	-1.155500
7	-2.826380	3.751163	1.545365
7	2.161836	3.380828	-1.094891
7	-3.035904	1.378888	-2.293120
7	-1.477270	0.985524	0.508998
7	1.776620	0.596035	0.622956
7	0.435362	3.337791	1.613649

7	5.369234	2.965225	-0.962504
7	3.691298	3.026997	1.683153
7	-3.690588	-3.914842	-2.725250
7	-0.368048	-4.301659	-2.623617
7	2.919167	-4.762793	-2.406180
8	-3.007513	-1.177000	4.586442
8	-0.668205	-2.608399	4.607490
8	2.481259	-5.089642	3.025426
8	-3.625036	-4.397212	2.709702
8	-0.686618	-4.731253	2.806327
8	-5.420301	-2.405191	3.824877
8	-3.315526	1.056500	3.153594
8	-0.039451	0.460464	3.261527
8	1.225643	0.143974	6.205102
8	3.446116	0.657531	3.490777
8	-0.974018	2.992151	4.623578
8	1.873896	2.549284	4.843557
8	-1.520908	0.753566	6.174318
31	-5.064764	-0.611265	0.292671
31	-5.398215	-3.077476	-1.925836
31	-3.240130	-0.587728	-2.619781
31	0.026450	-0.996389	-2.505566
31	3.278165	-1.416248	-2.367954
31	4.857171	-1.799143	0.662274
31	-3.673322	-3.531663	1.050605
31	-1.736443	-0.961103	0.282174
31	1.542747	-1.354577	0.427108
31	-1.990350	-3.417679	-1.785368
31	1.333419	-3.832670	-1.610713
31	-0.486662	-3.949128	1.103306
31	4.717855	-4.339615	-1.491460
31	2.740718	-4.282752	1.354185
31	-4.688665	2.215617	-1.463926
31	-4.409145	4.767592	0.728169
31	1.947167	1.446030	-1.218820
31	5.270148	0.989746	-1.156177
31	-1.088417	4.387701	0.735413
31	-1.358138	1.857337	-1.324276
31	-3.041992	1.801155	1.418548
31	0.204373	1.403295	1.445295
31	3.431487	1.076154	1.632302
31	2.193486	4.013734	0.783505
31	5.506477	3.612196	0.957144
31	3.887427	3.949300	-1.979970
31	0.639866	4.327427	-2.054427
31	-2.590230	4.767207	-2.115536

8	0.851103	-0.482934	3.413798
1	-0.065888	-1.913476	4.309284

-NH Deprotonation TS Structure (doublet) in Scheme S2

E = -2611.03270371 a.u.

1	-3.461759	-1.232393	2.090404
1	-1.060449	0.445673	3.296724
1	-0.669961	-1.856796	2.688153
1	-0.790775	-1.708818	4.401132
1	-0.859481	-3.164668	3.602068
1	1.495507	-5.102685	3.148307
1	-4.530476	-3.791019	3.247755
1	2.965277	-2.097167	2.370430
1	-1.175518	-5.159848	3.042778
1	-5.940051	-2.097308	2.736766
1	-5.153334	-1.850756	4.008822
1	-2.796845	1.734538	3.777539
1	-3.440673	-0.335447	4.155120
1	-3.071167	-1.798358	4.319525
1	0.218793	1.609202	7.164370
1	1.253080	1.570980	6.053082
1	2.308696	-0.116829	3.471276
1	-0.567102	2.192297	4.145587
1	-0.772704	2.909400	5.471922
1	1.321629	2.930483	4.509513
1	2.429042	1.885520	4.300797
1	-0.362820	-0.232184	5.994520
1	-1.803449	-0.740441	5.767187
1	3.600626	3.228889	2.753533
1	-2.747028	4.020150	2.518562
1	0.405988	3.633229	2.580497
1	-4.027005	6.405257	0.769875
1	6.252318	3.228663	-1.291382
1	6.646503	2.765814	1.864819
1	2.379353	5.594805	0.989911
1	-0.850529	5.998979	0.875851
1	-5.417274	1.822639	0.871408
1	-6.452017	-0.984885	0.960928
1	-5.652688	-0.618211	-2.139886
1	-5.982753	1.929689	-2.303128
1	-5.416904	-4.875486	-0.121698
1	1.023060	-5.660777	0.099207
1	5.978623	-5.065122	-2.167075

1	5.145297	-5.079757	0.973911
1	6.019062	-2.581312	1.529462
1	5.746845	0.389841	1.361477
1	6.576111	0.295346	-1.754541
1	5.624613	-2.088407	-1.630374
1	-3.218046	-1.012045	-4.159545
1	-2.902264	1.805957	-3.236706
1	0.062052	-1.452700	-4.047929
1	0.388856	1.374874	-3.111053
1	3.406704	-1.878548	-3.874525
1	3.657557	0.950093	-2.936568
1	-6.700570	-3.414054	-2.738070
1	-6.161723	-3.577134	0.483284
1	-2.284899	-5.241895	0.024595
1	-5.730263	4.306525	1.389977
1	5.557556	5.199977	1.098707
1	-4.984529	4.693720	-1.718241
1	4.142749	-6.147887	0.289452
1	3.986053	3.397007	-3.478206
1	4.145104	5.523686	-1.709123
1	0.706967	3.797284	-3.639229
1	0.889962	5.932011	-1.892733
1	-2.589706	4.289373	-3.731214
1	-2.357328	6.390362	-1.940765
1	-3.808920	-4.946507	-2.623563
1	-3.603874	-3.717349	-3.657645
1	-0.318926	-4.075543	-3.557753
1	-0.496794	-5.349387	-2.568464
1	3.025584	-4.553233	-3.389184
1	2.783272	-5.782568	-2.364085
7	-4.916809	-1.138993	-1.653096
7	-5.325951	-3.862648	-0.029874
7	1.555537	-1.933268	-1.470746
7	4.738433	-2.396611	-1.218983
7	2.999313	-2.380571	1.386041
7	-2.143365	-4.233002	0.123987
7	-1.713144	-1.528475	-1.607124
7	-3.473689	-1.516968	1.106737
7	-0.240420	-1.954920	1.180546
7	1.141647	-4.649696	0.202635
7	4.307060	-5.145796	0.394599
7	-4.641542	1.387379	0.364683
7	-4.245448	4.184078	-1.226657
7	0.279866	0.951769	-2.184379
7	3.556796	0.528055	-2.009030
7	4.927698	0.159505	0.791859

7	-1.056379	3.781928	-1.192686
7	-2.786391	3.771943	1.526020
7	2.182232	3.353173	-1.057609
7	-3.000442	1.387637	-2.307022
7	-1.472762	1.002597	0.469121
7	1.750782	0.579819	0.639268
7	0.436106	3.349876	1.597150
7	5.375589	2.935429	-0.852152
7	3.663024	2.963178	1.766550
7	-3.686849	-3.933452	-2.663442
7	-0.375852	-4.335739	-2.572153
7	2.941454	-4.774282	-2.396374
8	-3.596025	-1.105398	4.739459
8	-1.116937	-2.188779	3.582531
8	2.454627	-5.155303	3.019208
8	-3.816319	-4.268063	2.798122
8	-0.442791	-4.545515	2.928357
8	-5.872342	-2.398180	3.649570
8	-3.165867	1.083107	3.170117
8	-0.127908	0.708546	3.284377
8	0.758872	0.993685	6.660956
8	3.106093	0.424940	3.485128
8	-0.754038	3.074694	4.524215
8	2.169543	2.637857	4.869089
8	-0.889066	-1.042038	5.860711
31	-5.053403	-0.563006	0.279139
31	-5.390529	-3.044618	-1.912842
31	-3.205405	-0.585000	-2.600827
31	0.053627	-1.026987	-2.486386
31	3.312911	-1.436652	-2.322862
31	4.838897	-1.838288	0.724304
31	-3.701580	-3.473859	1.112901
31	-1.704090	-0.952740	0.331165
31	1.503825	-1.377928	0.473505
31	-1.990065	-3.451089	-1.717113
31	1.349575	-3.853674	-1.603267
31	-0.448995	-3.901769	1.118995
31	4.736196	-4.359922	-1.464485
31	2.743425	-4.334132	1.363906
31	-4.636567	2.252625	-1.474939
31	-4.342853	4.814372	0.702047
31	1.969063	1.409586	-1.179211
31	5.287226	0.959099	-1.046370
31	-1.049589	4.402795	0.693055
31	-1.305075	1.847198	-1.336183
31	-3.007967	1.818289	1.403528

31	0.179672	1.384167	1.518572
31	3.375973	1.016913	1.688297
31	2.199396	3.995082	0.818768
31	5.480245	3.578364	1.067669
31	3.935766	3.922351	-1.935920
31	0.712205	4.318954	-2.092505
31	-2.521898	4.786809	-2.179277

-N$^{\bullet-}$ Structure (doublet) in Scheme S2

E = -2610.61095071 a.u.

1	-3.507894	-1.135354	2.068881
1	-0.431895	-0.259966	3.192910
1	-1.271527	-1.584642	4.681731
1	-1.204601	-2.726697	3.625437
1	1.323508	-5.112206	3.246889
1	-4.590160	-3.821647	3.208417
1	2.909915	-2.119992	2.378916
1	-1.869514	-4.578580	3.035027
1	-6.211473	-2.178582	2.531781
1	-5.408898	-1.867013	3.777362
1	-2.591930	1.746469	3.781121
1	-3.868072	-0.106616	4.074200
1	-3.317756	-1.485691	4.320066
1	1.267519	0.637089	7.297145
1	1.595374	1.188166	5.924503
1	2.127302	0.082483	3.438822
1	-0.495763	1.735719	4.182922
1	-0.820203	2.331589	5.550307
1	1.276963	2.745466	4.585252
1	2.507337	1.890238	4.264866
1	-0.461643	0.027281	6.079550
1	-1.838164	0.241029	5.463695
1	3.792111	3.100708	2.747872
1	-2.604680	4.109449	2.536051
1	0.575838	3.561803	2.624247
1	-3.789980	6.537890	0.787789
1	6.407474	2.974293	-1.314692
1	6.809767	2.509132	1.831939
1	2.547164	5.487060	1.042597
1	-0.564288	5.987955	0.945311
1	-5.358557	1.994726	0.882243
1	-6.509830	-0.767245	0.922807
1	-5.680492	-0.423114	-2.155499

1	-5.911763	2.133205	-2.280866
1	-5.561621	-4.712677	-0.182799
1	0.853734	-5.687997	0.164385
1	5.772169	-5.318198	-2.089334
1	4.924715	-5.262447	1.038034
1	5.963336	-2.802255	1.517087
1	5.792024	0.194651	1.342193
1	6.593573	0.032739	-1.761586
1	5.552314	-2.317674	-1.629286
1	-3.294072	-0.861669	-4.192810
1	-2.834870	1.932054	-3.212831
1	0.029932	-1.441582	-4.054300
1	0.412643	1.385016	-3.111651
1	3.356270	-2.027879	-3.883589
1	3.722086	0.806741	-2.970856
1	-6.812690	-3.179744	-2.768093
1	-6.296541	-3.416319	0.439702
1	-2.483776	-5.146208	-0.051902
1	-5.570790	4.516341	1.425827
1	5.812901	4.980997	1.084434
1	-4.825870	4.853757	-1.692264
1	3.856240	-6.267513	0.358838
1	4.131105	3.308938	-3.467069
1	4.399605	5.384926	-1.669042
1	0.837637	3.816206	-3.601778
1	1.120986	5.910739	-1.839858
1	-2.424045	4.409011	-3.685962
1	-2.126155	6.466338	-1.870563
1	-3.957742	-4.784131	-2.670583
1	-3.725223	-3.551590	-3.694042
1	-0.407547	-4.038267	-3.546748
1	-0.684514	-5.303800	-2.568936
1	2.839341	-4.677334	-3.329004
1	2.552125	-5.891821	-2.297237
7	-4.958103	-0.964577	-1.671156
7	-5.459667	-3.702840	-0.070749
7	1.496621	-1.980883	-1.478619
7	4.652214	-2.572941	-1.211630
7	2.939709	-2.441789	1.406611
7	-2.298643	-4.146816	0.069301
7	-1.768503	-1.436266	-1.628450
7	-3.538910	-1.414132	1.084524
7	-0.277279	-1.988463	0.963265
7	0.960323	-4.675660	0.272939
7	4.083943	-5.277096	0.458940
7	-4.590656	1.538557	0.382001

7	-4.098363	4.326357	-1.203633
7	0.320504	0.959820	-2.184132
7	3.590080	0.399072	-2.040889
7	4.956826	-0.014324	0.788181
7	-0.903681	3.821361	-1.159237
7	-2.638032	3.872137	1.541019
7	2.337487	3.294520	-1.054450
7	-2.939080	1.500573	-2.289890
7	-1.437452	1.047876	0.509101
7	1.815850	0.540352	0.592266
7	0.576574	3.282205	1.639800
7	5.516535	2.733085	-0.874014
7	3.822214	2.840093	1.758771
7	-3.810345	-3.774170	-2.701582
7	-0.512993	-4.297549	-2.564975
7	2.750862	-4.891024	-2.334886
8	-4.084528	-0.935625	4.544009
8	-1.526489	-1.821475	3.774356
8	2.277385	-5.148129	3.104414
8	-3.872006	-4.245064	2.715886
8	-0.910645	-4.462609	2.940356
8	-6.094530	-2.474074	3.440781
8	-3.244681	1.305305	3.220910
8	0.183842	0.487282	3.226888
8	1.284165	0.382655	6.369712
8	3.067313	0.325245	3.453218
8	-0.810046	2.560038	4.614701
8	2.191019	2.595085	4.862220
8	-1.370789	-0.322788	6.088685
31	-5.087392	-0.388912	0.265699
31	-5.491147	-2.848427	-1.944019
31	-3.225786	-0.454423	-2.631138
31	0.023258	-1.003483	-2.496013
31	3.277005	-1.558692	-2.339616
31	4.810896	-2.003665	0.729032
31	-3.827747	-3.360860	1.066599
31	-1.783454	-0.865707	0.286049
31	1.550101	-1.382896	0.424134
31	-2.102247	-3.340034	-1.745957
31	1.199622	-3.892118	-1.551195
31	-0.644436	-3.932246	1.158549
31	4.560283	-4.538676	-1.410737
31	2.570894	-4.371598	1.424655
31	-4.550581	2.408910	-1.457342
31	-4.164769	4.955635	0.727107
31	2.041637	1.370993	-1.216957

31	5.332665	0.763546	-1.063731
31	-0.867608	4.406215	0.737546
31	-1.237608	1.904921	-1.316881
31	-2.951273	1.930126	1.436956
31	0.252103	1.338666	1.509657
31	3.439883	0.910398	1.674079
31	2.359213	3.886195	0.844492
31	5.660708	3.360582	1.050593
31	4.097964	3.794404	-1.903629
31	0.869860	4.299722	-2.033975
31	-2.343811	4.863913	-2.115763