

Table S1. Calculated and experimental $L_b - S_0$ transition energies (eV) for 1-NpOH-(NH₃)_n ($n = 0-5$) clusters

	$L_b - S_0$ (calculated)	$L_b - S_0$ (experimental)
<i>trans</i> -1-NpOH	4.47	3.90
1-NpOH-(NH ₃) ₁	4.42	3.87
1-NpOH-(NH ₃) ₂	4.41	3.87
1-NpOH-(NH ₃) ₃	4.39	3.86
1-NpOH-(NH ₃) ₄	4.39	3.85
1-NpOH-(NH ₃) ₅	4.38	3.63

Table S2. Calculated XYZ coordinates (Å) of all the 1-NpOH-(NH₃)_n (n = 0-5) clusters in the S₀, L_b and L_a states

(Oa)

Ground state optimized

Atom	X	Y	Z
C	-1.401070	0.674586	0.000000
C	-2.291085	-0.364136	0.000000
C	-1.824764	-1.695745	0.000000
C	-0.488616	-1.968517	0.000000
C	0.453099	-0.909641	0.000000
C	1.848188	-1.148250	0.000000
C	2.737787	-0.111468	0.000000
C	2.278055	1.222446	0.000000
C	0.937808	1.490101	0.000000
C	0.000000	0.432484	0.000000
O	-1.785602	1.979409	0.000000
H	-2.745077	2.028758	0.000000
H	-3.355487	-0.162168	0.000000
H	-2.545320	-2.502130	0.000000
H	-0.130267	-2.989215	0.000000
H	2.197271	-2.173066	0.000000
H	3.800956	-0.310261	0.000000
H	2.992296	2.034331	0.000000
H	0.574031	2.507326	0.000000

(Oa)

Lb state optimized

Atom	X	Y	Z
C	1.345134	0.792149	-0.031295
C	2.353500	-0.170226	-0.014468
C	2.006410	-1.546349	0.036904
C	0.674754	-1.929752	0.059808
C	-0.386481	-0.967337	0.002705
C	-1.753732	-1.334076	-0.096165
C	-2.739913	-0.337703	-0.052650

C	-2.400964	1.045928	0.030925
C	-1.077092	1.451018	0.119892
C	-0.048949	0.447721	0.042636
O	1.601310	2.114015	-0.076666
H	2.559998	2.249778	-0.090578
H	3.400110	0.142638	-0.036755
H	2.794748	-2.298615	0.053059
H	0.408100	-2.987487	0.097805
H	-2.023196	-2.388708	-0.149927
H	-3.792588	-0.626518	-0.050586
H	-3.199387	1.789062	0.022007
H	-0.794263	2.499495	0.178554

(Oa)

La state optimized

Atom	X	Y	Z
C	-1.406911	0.638637	0.000000
C	-2.340905	-0.451958	0.000000
C	-1.856287	-1.733443	0.000000
C	-0.446631	-1.954817	0.000000
C	0.491203	-0.898324	0.000000
C	1.883184	-1.117089	0.000000
C	2.791851	-0.015340	0.000000
C	2.311633	1.273183	0.000000
C	0.904365	1.528086	0.000000
C	0.000000	0.451758	0.000000
O	-1.850057	1.906377	0.000000
H	-2.817890	1.908700	0.000000
H	-3.411759	-0.238671	0.000000
H	-2.536073	-2.584732	0.000000
H	-0.074115	-2.980864	0.000000
H	2.258411	-2.140754	0.000000
H	3.865232	-0.204897	0.000000
H	3.001413	2.117903	0.000000
H	0.526215	2.548140	0.000000

(Ob)

Ground state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-1.362963	0.78037	0.000001
C	-2.322459	-0.195441	-0.000004
C	-1.954793	-1.553097	-0.000005
C	-0.640384	-1.922984	0.000001
C	0.372462	-0.936297	0.000003
C	1.744633	-1.286542	0.000004
C	2.719495	-0.331352	0.000001
C	2.368844	1.034656	-0.000005
C	1.054451	1.407156	-0.000004
C	0.02011	0.43979	0.000001
O	-1.782155	2.072836	0.000004
H	-1.030636	2.668503	0.000029
H	-3.361261	0.102358	-0.000006
H	-2.731372	-2.305742	-0.000008
H	-0.35482	-2.966282	0.000004
H	2.005438	-2.337299	0.000008
H	3.762456	-0.616603	0.000002
H	3.14385	1.788444	-0.000011
H	0.827207	2.466376	-0.000011

(Ob)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-1.362451	0.799183	0.010943
C	-2.363091	-0.186955	-0.017105
C	-1.999055	-1.557478	-0.041886
C	-0.649282	-1.929712	-0.014492
C	0.383870	-0.966625	0.019687
C	1.751559	-1.311988	0.053498
C	2.755042	-0.342362	0.032785
C	2.404205	1.037544	-0.044764
C	1.061780	1.421237	-0.068547
C	0.022256	0.471698	-0.002945

O	-1.786033	2.078814	0.051597
H	-1.029626	2.658193	0.214714
H	-3.402923	0.134183	-0.000610
H	-2.775354	-2.320869	-0.066913
H	-0.376640	-2.986650	-0.022403
H	2.017409	-2.370565	0.088436
H	3.803090	-0.637083	0.061432
H	3.183978	1.796628	-0.093126
H	0.839332	2.488401	-0.157355

(Ob)

La state optimized

Atom	X	Y	Z
C	-1.323898	0.811301	-0.002843
C	-2.395510	-0.139971	-0.044819
C	-2.084238	-1.474357	-0.043812
C	-0.717540	-1.873732	-0.002791
C	0.356168	-0.952170	0.011867
C	1.707939	-1.357362	0.068706
C	2.745939	-0.380880	0.056890
C	2.450332	0.958346	-0.044175
C	1.089158	1.394741	-0.128778
C	0.050532	0.444754	-0.049832
O	-1.685158	2.089131	0.125361
H	-0.891385	2.610338	0.335287
H	-3.416270	0.239406	-0.052082
H	-2.868106	-2.230146	-0.068292
H	-0.479867	-2.939401	-0.005966
H	1.944849	-2.418455	0.140000
H	3.784585	-0.706306	0.123619
H	3.249489	1.699304	-0.068980
H	0.884678	2.448195	-0.328960

(Ia)

Ground state optimized

Atom	X	Y	Z
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C	-0.615750	-0.722738	0.000000
C	0.162023	-1.854393	0.000000
C	1.568424	-1.753140	0.000000
C	2.188332	-0.537704	0.000000
C	1.413950	0.648774	0.000000
C	2.010627	1.932573	0.000000
C	1.244890	3.064156	0.000000
C	-0.162956	2.971389	0.000000
C	-0.771890	1.747386	0.000000
C	0.000000	0.563637	0.000000
O	-1.961692	-0.749109	0.000000
H	-2.293848	-1.673561	0.000000
H	-0.312434	-2.826687	0.000000
H	2.157088	-2.661011	0.000000
H	3.267539	-0.462162	0.000000
H	3.091388	1.999836	0.000000
H	1.716910	4.037537	0.000000
H	-0.758908	3.873868	0.000000
H	-1.848671	1.659643	0.000000
N	-3.099416	-3.334313	0.000000
H	-4.102493	-3.191485	0.000000
H	-2.876508	-3.891276	0.816283
H	-2.876508	-3.891276	-0.816283

(Ia)

Lb state optimized

Atom	X	Y	Z
C	-0.709116	-0.656704	0.000000
C	-0.024404	-1.893034	0.000000
C	1.395404	-1.924166	0.000000
C	2.122830	-0.725825	0.000000
C	1.477133	0.530043	0.000000
C	2.178398	1.758000	0.000000
C	1.510110	2.980609	0.000000
C	0.083027	3.018929	0.000000
C	-0.646009	1.827337	0.000000

C	0.000000	0.579972	0.000000
O	-2.040532	-0.593153	0.000000
H	-2.437614	-1.506044	0.000000
H	-0.601318	-2.817288	0.000000
H	1.915381	-2.881114	0.000000
H	3.214503	-0.753181	0.000000
H	3.270590	1.733809	0.000000
H	2.079441	3.909978	0.000000
H	-0.435937	3.976774	0.000000
H	-1.736096	1.845557	0.000000
N	-3.267371	-3.070478	0.000000
H	-4.281252	-2.942844	0.000000
H	-3.058041	-3.649023	0.816034
H	-3.058041	-3.649023	-0.816034

(Ia)

La state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-0.657351	-0.684820	0.000000
C	0.070834	-1.928886	0.000000
C	1.441263	-1.899291	0.000000
C	2.115846	-0.645269	0.000000
C	1.432786	0.593738	0.000000
C	2.110018	1.832198	0.000000
C	1.371390	3.053158	0.000000
C	-0.004399	3.031971	0.000000
C	-0.717063	1.792402	0.000000
C	0.000000	0.582073	0.000000
O	-1.980691	-0.684617	0.000000
H	-2.350249	-1.615640	0.000000
H	-0.488410	-2.864241	0.000000
H	2.018623	-2.823369	0.000000
H	3.207765	-0.633951	0.000000
H	3.200049	1.842937	0.000000
H	1.906213	4.003504	0.000000
H	-0.567223	3.966501	0.000000

H	-1.804314	1.771898	0.000000
N	-3.162367	-3.152579	0.000000
H	-4.171563	-2.990090	0.000000
H	-2.974371	-3.738103	0.816464
H	-2.974371	-3.738103	-0.816464

(Ib)

Ground state optimized

Atom	X	Y	Z
C	0.941812	-0.975719	-0.394250
C	0.611184	-2.285362	-0.161359
C	-0.693441	-2.636493	0.234733
C	-1.654060	-1.681710	0.412687
C	-1.354549	-0.322369	0.161088
C	-2.328580	0.695650	0.310589
C	-2.038712	1.998312	0.021934
C	-0.756362	2.350051	-0.452194
C	0.210113	1.394142	-0.596791
C	-0.052332	0.041011	-0.271267
O	2.205782	-0.668065	-0.771761
H	1.380135	-3.036279	-0.276073
H	-0.924825	-3.677771	0.415161
H	-2.651959	-1.948363	0.734926
H	-3.317143	0.415888	0.652738
H	-2.795441	2.762330	0.137789
H	-0.546927	3.377567	-0.717407
H	1.181643	1.656589	-0.991820
N	3.001530	1.352227	1.004054
H	3.417664	2.219845	0.688415
H	3.626585	0.947549	1.690626
H	2.136316	1.588659	1.477576
H	2.526555	0.107854	-0.257241

(Ib)

Lb state optimized

Atom	X	Y	Z
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C	0.756205	-1.168802	-0.322747
C	0.137713	-2.424350	-0.158231
C	-1.241784	-2.501702	0.163311
C	-1.991027	-1.332581	0.346140
C	-1.415595	-0.051572	0.181258
C	-2.146807	1.145253	0.335936
C	-1.589943	2.388929	0.036342
C	-0.262115	2.462659	-0.483716
C	0.500425	1.301940	-0.627470
C	0.002157	0.042709	-0.236891
O	2.068806	-1.156365	-0.569917
H	0.761897	-3.313240	-0.234337
H	-1.711159	-3.475313	0.299501
H	-3.048823	-1.400055	0.608937
H	-3.182418	1.080620	0.677800
H	-2.177972	3.297174	0.163090
H	0.149289	3.424651	-0.789468
H	1.496314	1.362442	-1.070005
N	3.184366	0.865645	0.885847
H	3.706689	1.650346	0.492070
H	3.788402	0.449320	1.596926
H	2.391887	1.279302	1.383696
H	2.489511	-0.338739	-0.173395

(Ib)

La state optimized

Atom	X	Y	Z
C	-0.716475	1.157249	-0.301824
C	-0.092227	2.448950	-0.174670
C	1.236762	2.523549	0.151735
C	1.972294	1.323114	0.333689
C	1.407005	0.035342	0.153872
C	2.169860	-1.146603	0.306886
C	1.579826	-2.412588	0.028310
C	0.275602	-2.499625	-0.401229
C	-0.522644	-1.320750	-0.549507

C	0.034748	-0.059210	-0.233888
O	-2.022603	1.174021	-0.470996
H	-0.728858	3.324011	-0.299707
H	1.729134	3.487096	0.278258
H	3.032892	1.385728	0.586396
H	3.210076	-1.073761	0.622497
H	2.176058	-3.318144	0.148396
H	-0.160137	-3.471665	-0.637190
H	-1.507693	-1.378738	-1.010397
N	-3.276643	-0.811805	0.764810
H	-3.867153	-1.474924	0.258997
H	-3.838047	-0.454123	1.540127
H	-2.512889	-1.363072	1.167146
H	-2.484566	0.331487	-0.120458

(IIa)

Ground state optimized

Atom	X	Y	Z
C	-0.700644	0.037996	-0.682808
C	-1.183803	1.320347	-0.580607
C	-0.339633	2.368494	-0.159116
C	0.970294	2.139945	0.150632
C	1.501923	0.830979	0.045592
C	2.853493	0.543615	0.354166
C	3.342214	-0.728492	0.255869
C	2.502517	-1.784414	-0.157781
C	1.192560	-1.542044	-0.465186
C	0.665304	-0.233437	-0.372593
O	-1.462157	-1.010159	-1.045295
H	-2.217083	1.518570	-0.830111
H	-0.746188	3.368579	-0.086582
H	1.616059	2.946423	0.471580
H	3.495125	1.356240	0.671106
H	4.377682	-0.930860	0.494596
H	2.901103	-2.786923	-0.233205
H	0.538655	-2.338262	-0.791001

H	-2.424165	-0.783651	-0.948672
N	-4.037371	-0.515555	-0.258385
H	-3.697844	-0.481084	0.705128
H	-4.658999	-1.310367	-0.342460
H	-4.586860	0.315688	-0.435591
N	-2.055330	-0.676758	2.083298
H	-2.006344	-0.989741	3.045033
H	-1.517134	0.181057	2.019240
H	-1.553209	-1.356142	1.519901

(IIa)

Lb state optimized

Atom	X	Y	Z
C	-0.733183	0.009435	-0.698661
C	-1.263846	1.316804	-0.585720
C	-0.431405	2.387590	-0.164360
C	0.917058	2.156164	0.142636
C	1.487612	0.867637	0.040449
C	2.837537	0.593932	0.356151
C	3.364236	-0.692576	0.259627
C	2.534049	-1.775048	-0.164923
C	1.194239	-1.546955	-0.482429
C	0.635356	-0.258560	-0.396748
O	-1.491913	-1.021432	-1.057961
H	-2.304453	1.488600	-0.857156
H	-0.841799	3.394146	-0.092461
H	1.550660	2.985862	0.463204
H	3.472624	1.419906	0.684746
H	4.410323	-0.872675	0.505831
H	2.949536	-2.779072	-0.245843
H	0.555787	-2.366909	-0.813293
H	-2.472188	-0.792551	-0.928669
N	-3.948937	-0.559410	-0.183488
H	-3.544926	-0.552689	0.768380
H	-4.598719	-1.345807	-0.228686
H	-4.513594	0.284832	-0.283530

N	-1.949817	-0.704429	2.053206
H	-1.897854	-1.006374	3.027768
H	-1.424397	0.173517	2.009074
H	-1.364346	-1.362999	1.530167

(IIa)

La state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-0.780618	0.115226	-0.747402
C	-1.349300	1.424345	-0.534806
C	-0.556255	2.426686	-0.036887
C	0.805272	2.152430	0.271447
C	1.399229	0.881550	0.073852
C	2.743205	0.610807	0.416627
C	3.282792	-0.691649	0.207380
C	2.499126	-1.700305	-0.304659
C	1.127140	-1.462147	-0.634790
C	0.591542	-0.171328	-0.461547
O	-1.536536	-0.873927	-1.175172
H	-2.389724	1.589177	-0.814174
H	-0.954238	3.429394	0.116196
H	1.427200	2.955170	0.673522
H	3.355337	1.404155	0.845409
H	4.326899	-0.883903	0.457693
H	2.920410	-2.693207	-0.467597
H	0.505364	-2.247525	-1.059249
H	-2.518652	-0.703441	-0.914129
N	-3.816168	-0.629177	0.039839
H	-3.262430	-0.763883	0.905558
H	-4.461731	-1.416865	-0.033168
H	-4.389692	0.205901	0.164175
N	-1.530965	-1.081685	1.937802
H	-1.467599	-1.542029	2.848104
H	-0.980115	-0.223236	2.035164
H	-0.961601	-1.655951	1.305093

(IIb)

Ground state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.954332	-1.021921	-0.644145
C	0.748075	-2.316080	-0.235237
C	-0.501481	-2.720402	0.272161
C	-1.535105	-1.833163	0.387884
C	-1.365371	-0.494418	-0.036939
C	-2.403906	0.462978	0.080576
C	-2.224941	1.751766	-0.336438
C	-0.999617	2.145559	-0.918755
C	0.023483	1.247400	-1.041656
C	-0.120923	-0.083425	-0.582493
O	2.163307	-0.653586	-1.114224
H	1.574123	-3.010229	-0.298976
H	-0.631935	-3.746652	0.589042
H	-2.489618	-2.138815	0.795564
H	-3.347911	0.150148	0.509014
H	-3.027290	2.470574	-0.238825
H	-0.879173	3.158611	-1.277650
H	0.955955	1.537933	-1.504020
N	2.871942	1.459378	0.458449
H	2.158868	1.376789	1.189256
H	2.861428	2.415742	0.125984
H	3.776021	1.300108	0.886320
H	2.457573	0.182375	-0.654454
N	0.475429	0.886168	2.355498
H	0.356981	-0.112817	2.219312
H	0.347043	1.071863	3.342764
H	-0.297387	1.324478	1.863091

(IIb)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-0.150255	1.480306	-0.505126
C	0.845040	2.405273	-0.120916

C	2.118828	1.947875	0.305138
C	2.383822	0.575780	0.393527
C	1.418631	-0.390638	0.019060
C	1.650377	-1.780749	0.093223
C	0.727916	-2.704249	-0.401273
C	-0.461091	-2.241058	-1.048251
C	-0.731628	-0.874122	-1.120172
C	0.129077	0.074616	-0.537252
O	-1.346633	1.950774	-0.830006
H	0.581039	3.461664	-0.114975
H	2.880830	2.667989	0.601601
H	3.358828	0.231577	0.745720
H	2.589075	-2.129742	0.530436
H	0.934245	-3.772096	-0.336375
H	-1.147242	-2.956900	-1.500709
H	-1.623532	-0.524202	-1.641996
N	-3.147668	0.428644	0.331987
H	-2.575656	-0.035911	1.062838
H	-3.675209	-0.310199	-0.135521
H	-3.835519	1.009120	0.815138
H	-2.084155	1.304179	-0.515799
N	-1.127436	-0.809877	2.195307
H	-0.388969	-0.100286	2.202218
H	-1.163928	-1.177954	3.147716
H	-0.735320	-1.563007	1.620945

(IIb)

La state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-1.254065	-0.788153	-0.504678
C	-2.570638	-0.326395	-0.136614
C	-2.729328	0.950306	0.340526
C	-1.595413	1.796394	0.441200
C	-0.299719	1.410067	0.005088
C	0.818230	2.276539	0.094712
C	2.078368	1.857381	-0.424483

C	2.215786	0.627851	-1.033445
C	1.104353	-0.265569	-1.128241
C	-0.133998	0.109932	-0.559059
O	-1.128266	-2.062048	-0.761119
H	-3.385544	-1.046709	-0.202291
H	-3.708128	1.314382	0.651340
H	-1.723662	2.809172	0.829507
H	0.699271	3.261346	0.545155
H	2.936371	2.527384	-0.350958
H	3.179321	0.329089	-1.449554
H	1.186179	-1.203706	-1.673794
N	0.984542	-2.961020	0.330467
H	1.187703	-2.228962	1.044946
H	1.836648	-3.071542	-0.220937
H	0.825893	-3.843520	0.820424
H	-0.174645	-2.449272	-0.425129
N	1.349764	-0.624008	2.126631
H	0.411144	-0.220624	2.197070
H	1.770135	-0.500960	3.049512
H	1.843845	0.025383	1.503939

(IIc)

Ground state optimized

Atom	X	Y	Z
C	-0.644954	-0.563696	-0.015236
C	-0.736947	-1.931564	0.038213
C	0.428543	-2.723924	0.083131
C	1.666140	-2.151173	0.074849
C	1.793116	-0.740873	0.020294
C	3.059254	-0.108471	0.009425
C	3.163771	1.252620	-0.044147
C	2.003656	2.053450	-0.089347
C	0.763182	1.477836	-0.081232
C	0.631522	0.070602	-0.025548
O	-1.732212	0.238403	-0.062106
H	-1.712207	-2.399986	0.046028

H	0.328139	-3.800349	0.124770
H	2.561098	-2.758133	0.109374
H	3.946357	-0.728440	0.044356
H	4.138887	1.721150	-0.051578
H	2.095927	3.130132	-0.130234
H	-0.122620	2.096632	-0.112419
H	-2.558680	-0.294927	-0.072837
N	-2.345927	3.324640	0.159751
H	-2.827868	3.652343	0.986935
H	-2.271660	2.314827	0.226182
H	-2.939230	3.529941	-0.633954
N	-4.209328	-1.100897	-0.096042
H	-4.925216	-0.384954	-0.135615
H	-4.390885	-1.659775	0.729277
H	-4.341260	-1.700731	-0.901814

(IIc)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-0.733183	0.009435	-0.698661
C	-1.263846	1.316804	-0.585720
C	-0.431405	2.387590	-0.164360
C	0.917058	2.156164	0.142636
C	1.487612	0.867637	0.040449
C	2.837537	0.593932	0.356151
C	3.364236	-0.692576	0.259627
C	2.534049	-1.775048	-0.164923
C	1.194239	-1.546955	-0.482429
C	0.635356	-0.258560	-0.396748
O	-1.491913	-1.021432	-1.057961
H	-2.304453	1.488600	-0.857156
H	-0.841799	3.394146	-0.092461
H	1.550660	2.985862	0.463204
H	3.472624	1.419906	0.684746
H	4.410323	-0.872675	0.505831
H	2.949536	-2.779072	-0.245843

H	0.555787	-2.366909	-0.813293
H	-2.472188	-0.792551	-0.928669
N	-3.948937	-0.559410	-0.183488
H	-3.544926	-0.552689	0.768380
H	-4.598719	-1.345807	-0.228686
H	-4.513594	0.284832	-0.283530
N	-1.949817	-0.704429	2.053206
H	-1.897854	-1.006374	3.027768
H	-1.424397	0.173517	2.009074
H	-1.364346	-1.362999	1.530167

(IIc)

La state optimized

Atom	X	Y	Z
C	-0.780618	0.115226	-0.747402
C	-1.349300	1.424345	-0.534806
C	-0.556255	2.426686	-0.036887
C	0.805272	2.152430	0.271447
C	1.399229	0.881550	0.073852
C	2.743205	0.610807	0.416627
C	3.282792	-0.691649	0.207380
C	2.499126	-1.700305	-0.304659
C	1.127140	-1.462147	-0.634790
C	0.591542	-0.171328	-0.461547
O	-1.536536	-0.873927	-1.175172
H	-2.389724	1.589177	-0.814174
H	-0.954238	3.429394	0.116196
H	1.427200	2.955170	0.673522
H	3.355337	1.404155	0.845409
H	4.326899	-0.883903	0.457693
H	2.920410	-2.693207	-0.467597
H	0.505364	-2.247525	-1.059249
H	-2.518652	-0.703441	-0.914129
N	-3.816168	-0.629177	0.039839
H	-3.262430	-0.763883	0.905558
H	-4.461731	-1.416865	-0.033168

H	-4.389692	0.205901	0.164175
N	-1.530965	-1.081685	1.937802
H	-1.467599	-1.542029	2.848104
H	-0.980115	-0.223236	2.035164
H	-0.961601	-1.655951	1.305093

(IIIa)

Ground state optimized

Atom	X	Y	Z
C	-0.427137	0.070475	0.828711
C	-0.985733	1.319559	0.697803
C	-0.224018	2.391897	0.190949
C	1.078895	2.222400	-0.180603
C	1.687810	0.950848	-0.049253
C	3.035855	0.723633	-0.419868
C	3.603457	-0.512074	-0.289034
C	2.851173	-1.590223	0.224702
C	1.547641	-1.405432	0.593489
C	0.936905	-0.136410	0.462842
O	-1.103394	-0.999349	1.283253
H	-2.016312	1.473943	0.985537
H	-0.689284	3.365016	0.101520
H	1.660365	3.047636	-0.569502
H	3.610739	1.553960	-0.810526
H	4.634487	-0.668025	-0.576705
H	3.312132	-2.562951	0.329121
H	0.961788	-2.219765	0.995684
H	-2.086693	-0.809319	1.321162
N	-3.771870	-0.566136	1.089172
H	-3.791466	-0.166162	0.143625
H	-4.257238	0.065571	1.714269
H	-4.298048	-1.431337	1.073163
N	-1.012492	-1.814913	-1.736732
H	-1.078082	-1.994112	-0.738842
H	-1.049254	-2.708464	-2.211335
H	-0.083909	-1.436739	-1.888629

N	-3.176228	0.475520	-1.702303
H	-2.492215	-0.264659	-1.874389
H	-3.766501	0.541762	-2.522551
H	-2.648317	1.339101	-1.647014

(IIIa)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-1.054592	1.241765	-0.720090
C	-0.306362	2.364238	-0.277589
C	1.041090	2.224017	0.081410
C	1.698414	0.975326	0.006021
C	3.048235	0.790342	0.377940
C	3.665156	-0.457017	0.297575
C	2.927451	-1.587680	-0.171391
C	1.591450	-1.446422	-0.547769
C	0.941078	-0.200344	-0.473671
C	-0.435804	-0.027900	-0.814300
H	-2.100654	1.346026	-1.002298
H	-0.784345	3.342029	-0.222535
H	1.605094	3.093732	0.425008
H	3.611619	1.655163	0.736210
H	4.709210	-0.569242	0.588245
H	3.412443	-2.561001	-0.242290
H	1.026425	-2.304714	-0.913557
O	-1.104984	-1.109343	-1.195650
H	-2.115088	-0.919844	-1.261630
N	-3.699370	-0.682186	-1.103682
H	-3.769563	-0.243026	-0.161922
H	-4.169972	-0.064325	-1.766902
H	-4.250701	-1.541421	-1.077221
N	-3.315033	0.459954	1.585914
H	-2.545696	-0.185502	1.831497
H	-3.937433	0.477118	2.396294
H	-2.876740	1.383677	1.560762
N	-0.954761	-1.504372	1.904002

H	-0.991545	-1.909382	0.963921
H	-0.833924	-2.292080	2.542945
H	-0.061799	-1.004185	1.916228

(IIIa)

La state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-1.171687	1.172519	-0.833289
C	-0.487710	2.298020	-0.445117
C	0.877576	2.189293	-0.070621
C	1.586897	0.962250	-0.092462
C	2.933402	0.858794	0.331696
C	3.598531	-0.400135	0.276946
C	2.939160	-1.524220	-0.166118
C	1.568258	-1.454006	-0.570351
C	0.904765	-0.211849	-0.535466
C	-0.487615	-0.098223	-0.858033
H	-2.218096	1.209269	-1.133022
H	-0.978201	3.271175	-0.432242
H	1.412118	3.087507	0.246157
H	3.451010	1.747961	0.691011
H	4.641839	-0.466709	0.588877
H	3.458912	-2.482272	-0.211029
H	1.041858	-2.333301	-0.935086
O	-1.132646	-1.202374	-1.144907
H	-2.170941	-1.063405	-1.165203
N	-3.695899	-0.909268	-0.917170
H	-3.709683	-0.407614	-0.001628
H	-4.269978	-0.381217	-1.576196
H	-4.165339	-1.805983	-0.781281
N	-3.144127	0.438405	1.619953
H	-2.267338	-0.066477	1.842810
H	-3.711517	0.397410	2.469244
H	-2.862525	1.417766	1.532186
N	-0.535238	-1.130702	2.088149
H	-0.412708	-1.754542	1.283575

H	-0.438674	-1.731126	2.909901
H	0.317811	-0.563158	2.071545

(IIIb)

Ground state optimized

Atom	X	Y	Z
C	-0.725324	0.626635	-0.879410
C	-1.022740	1.913277	-0.501774
C	-0.066568	2.710291	0.157308
C	1.174829	2.220366	0.450985
C	1.523474	0.903896	0.065310
C	2.796298	0.354112	0.358730
C	3.119275	-0.917040	-0.024229
C	2.187698	-1.701487	-0.739739
C	0.949465	-1.202566	-1.033889
C	0.578153	0.099848	-0.623523
O	-1.657486	-0.124075	-1.500461
H	-2.010962	2.297046	-0.715932
H	-0.331038	3.720028	0.442111
H	1.905432	2.827173	0.969385
H	3.512007	0.965706	0.893684
H	4.095244	-1.322153	0.206822
H	2.461715	-2.697042	-1.060937
H	0.237291	-1.795932	-1.589052
N	-1.986245	-2.239319	0.081642
H	-1.333776	-2.079667	0.852192
H	-1.978396	-3.223516	-0.151595
H	-2.911729	-1.985035	0.419897
H	-1.727943	-1.020411	-1.033130
N	0.028699	-1.135877	2.236520
H	-0.121285	-0.135778	2.152859
H	0.112654	-1.344627	3.223950
H	0.934127	-1.313584	1.811700
N	-3.908752	0.057186	0.621006
H	-3.206226	0.510703	1.194930
H	-3.621446	0.220643	-0.339221

H -4.779049 0.551130 0.773228

(IIIb)

Lb state optimized

Atom	X	Y	Z
C	-0.781398	0.692381	-0.823505
C	-1.078460	2.018555	-0.429045
C	-0.095574	2.810826	0.219799
C	1.161630	2.270188	0.517568
C	1.507092	0.947620	0.148211
C	2.769969	0.377434	0.420521
C	3.117048	-0.890229	-0.046322
C	2.191843	-1.628772	-0.849870
C	0.930539	-1.101054	-1.128924
C	0.525636	0.142668	-0.610674
O	-1.737007	-0.033196	-1.380928
H	-2.082727	2.395282	-0.621269
H	-0.330812	3.833095	0.514337
H	1.906761	2.879926	1.033560
H	3.491971	0.962026	0.995946
H	4.101976	-1.302262	0.171495
H	2.479110	-2.597683	-1.257724
H	0.237144	-1.656582	-1.762165
N	-1.905925	-2.184833	-0.048896
H	-1.192337	-2.137882	0.700531
H	-1.955231	-3.145110	-0.387826
H	-2.803798	-1.939543	0.388116
H	-1.725739	-1.024442	-0.965378
N	0.179730	-1.531448	2.047179
H	0.071160	-0.513281	2.073403
H	0.311118	-1.818730	3.018726
H	1.087100	-1.666617	1.590791
N	-3.900831	-0.103306	0.726273
H	-3.269505	0.476817	1.285577
H	-3.692023	0.173637	-0.237258
H	-4.838884	0.246331	0.928119

(IIIb)

La state optimized

Atom	X	Y	Z
C	-1.047063	0.590207	-0.904810
C	-1.666898	1.761993	-0.302176
C	-0.948172	2.587759	0.537277
C	0.399318	2.294594	0.805655
C	1.080078	1.183152	0.211656
C	2.440782	0.893840	0.530354
C	3.105492	-0.145104	-0.188640
C	2.423974	-0.921536	-1.105391
C	1.032223	-0.724171	-1.350064
C	0.377502	0.361554	-0.691617
O	-1.748033	-0.247081	-1.534973
H	-2.714553	1.947885	-0.547251
H	-1.413747	3.463827	0.990683
H	0.965359	2.943769	1.476994
H	2.986590	1.545666	1.211733
H	4.170143	-0.317991	-0.018425
H	2.961758	-1.690798	-1.664941
H	0.514188	-1.248144	-2.152146
N	-1.185717	-2.357836	0.291511
H	-0.317448	-2.177425	0.923802
H	-1.310163	-3.358810	0.138919
H	-2.079174	-1.924262	0.659740
H	-1.015185	-1.887640	-0.618603
N	1.106348	-1.878785	1.724967
H	1.308750	-0.868976	1.673973
H	1.291464	-2.158147	2.690212
H	1.867035	-2.268859	1.159280
N	-3.514847	-0.855356	0.727863
H	-3.382596	-0.538845	-0.242184
H	-4.495719	-1.116429	0.835380
H	-3.376339	-0.018073	1.298766

(IIIc)

Ground state optimized

Atom	X	Y	Z
C	0.254780	0.363016	0.000000
C	-0.927623	1.067400	0.000000
C	-2.163773	0.386927	0.000000
C	-2.221998	-0.976710	0.000000
C	-1.023615	-1.732326	0.000000
C	-1.031775	-3.148109	0.000000
C	0.135551	-3.858022	0.000000
C	1.376797	-3.187153	0.000000
C	1.420750	-1.820690	0.000000
C	0.226184	-1.065127	0.000000
O	1.466958	0.942871	0.000000
H	-0.906466	2.148628	0.000000
H	-3.077060	0.967723	0.000000
H	-3.171862	-1.494619	0.000000
H	-1.986449	-3.659130	0.000000
H	0.111858	-4.939531	0.000000
H	2.294365	-3.759588	0.000000
H	2.362860	-1.291900	0.000000
H	1.411016	1.951663	0.000000
N	1.256131	3.615531	0.000000
H	2.061379	4.227437	0.000000
H	0.707777	3.794895	0.837824
H	0.707777	3.794895	-0.837824
N	0.135551	2.557658	-2.671536
H	0.794062	1.857849	-2.342192
H	-0.770211	2.102922	-2.671660
H	0.369571	2.751930	-3.637737
N	0.135551	2.557658	2.671536
H	0.794062	1.857849	2.342192
H	-0.770211	2.102922	2.671660
H	0.369571	2.751930	3.637737

(IIIc)

Lb state optimized

Atom	X	Y	Z
C	0.279159	-0.341390	-0.109603
C	0.979116	0.755179	0.461074
C	0.267209	1.881102	0.958447
C	-1.133961	1.908748	0.896844
C	-1.870154	0.837057	0.346480
C	-3.283598	0.834515	0.266394
C	-3.979983	-0.233458	-0.289842
C	-3.273719	-1.363896	-0.802431
C	-1.878898	-1.396805	-0.743212
C	-1.148938	-0.337566	-0.182055
O	0.912299	-1.408481	-0.571527
H	2.064346	0.703539	0.545302
H	0.812712	2.714172	1.400760
H	-1.677863	2.773014	1.284403
H	-3.828678	1.698742	0.653417
H	-5.068752	-0.206060	-0.335195
H	-3.822840	-2.197950	-1.237843
H	-1.326671	-2.251780	-1.134365
H	1.944566	-1.250369	-0.649668
N	3.480824	-1.014897	-0.662660
H	4.076520	-1.665143	-1.174796
H	3.702251	-1.099017	0.337395
H	3.702901	-0.058639	-0.976670
N	3.335499	1.878259	-1.624825
H	2.313401	1.813374	-1.593667
H	3.562832	2.696133	-1.055509
H	3.565087	2.146536	-2.583832
N	2.623368	-1.550841	2.166090
H	1.869820	-1.928745	1.583053
H	2.176542	-0.792925	2.687363
H	2.820199	-2.275590	2.859238

(IIIc)

La state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.303319	-0.250830	-0.858149
C	1.171565	0.902497	-0.805616
C	0.679024	2.101410	-0.348844
C	-0.675415	2.181067	0.073454
C	-1.563265	1.076537	0.028475
C	-2.900453	1.161338	0.480982
C	-3.745176	0.016915	0.416736
C	-3.268271	-1.182413	-0.062133
C	-1.911786	-1.303857	-0.500429
C	-1.074541	-0.173290	-0.465789
O	0.777793	-1.412440	-1.229050
H	2.192191	0.792234	-1.171850
H	1.305776	2.993761	-0.329244
H	-1.059994	3.135384	0.440124
H	-3.270724	2.104863	0.881858
H	-4.780258	0.098101	0.751755
H	-3.924936	-2.051907	-0.114354
H	-1.528686	-2.239906	-0.901598
H	1.820306	-1.477122	-0.987969
N	3.086852	-1.605606	-0.200146
H	3.697249	-2.402365	-0.381323
H	2.620875	-1.751228	0.710523
H	3.670742	-0.763293	-0.093795
N	4.186149	1.171743	0.529973
H	4.426391	1.933208	-0.108439
H	3.279933	1.434010	0.928414
H	4.855591	1.243940	1.298699
N	0.868242	-1.599507	1.849402
H	0.190862	-2.037548	1.213978
H	0.520545	-0.638371	1.925042
H	0.683090	-2.016896	2.763849

(III_d)

Ground state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
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C	-0.897885	-1.305484	-0.673360
C	-2.177266	-1.678209	-0.336218
C	-3.103867	-0.732635	0.140733
C	-2.755341	0.580619	0.295025
C	-1.453986	1.008279	-0.056291
C	-1.049190	2.358582	0.093495
C	0.206923	2.761308	-0.261010
C	1.123110	1.830690	-0.800127
C	0.769938	0.516725	-0.943945
C	-0.517275	0.068536	-0.562358
O	-0.027075	-2.225826	-1.120396
H	-2.446986	-2.720129	-0.436122
H	-4.101701	-1.060605	0.400767
H	-3.462925	1.305219	0.675708
H	-1.762147	3.069712	0.491669
H	0.498521	3.796685	-0.146975
H	2.100866	2.170984	-1.115967
H	1.464354	-0.198879	-1.362543
N	2.055743	-2.094624	0.548752
H	1.660435	-1.548987	1.317132
H	2.910204	-1.622259	0.259469
H	2.301132	-3.009401	0.906296
H	0.827578	-2.177504	-0.579544
N	0.440340	-0.140653	2.439036
H	-0.481503	-0.496565	2.205380
H	0.448002	0.036172	3.436253
H	0.510331	0.759124	1.973371
N	4.114220	0.161013	-0.130275
H	4.997918	0.346594	0.327610
H	4.197943	0.487007	-1.085638
H	3.411485	0.738828	0.318048

(IIIId)

Lb state optimized

Atom	X	Y	Z
C	-0.922697	-1.372415	-0.537220

C	-2.280080	-1.714620	-0.325466
C	-3.223392	-0.712176	0.008295
C	-2.822325	0.619136	0.163766
C	-1.476644	1.019246	-0.042373
C	-1.046767	2.353518	0.087149
C	0.250695	2.743421	-0.252694
C	1.153924	1.773123	-0.795060
C	0.769237	0.436849	-0.910656
C	-0.501097	0.002975	-0.486760
O	-0.064024	-2.339730	-0.770445
H	-2.549064	-2.768619	-0.371729
H	-4.264763	-0.984867	0.178936
H	-3.557772	1.380274	0.434391
H	-1.764577	3.099621	0.437359
H	0.556704	3.784197	-0.155373
H	2.132067	2.093148	-1.158617
H	1.454886	-0.292748	-1.345956
N	2.022029	-1.971698	0.642360
H	1.685056	-1.328238	1.380343
H	2.866828	-1.536127	0.245353
H	2.300290	-2.842417	1.096574
H	0.875702	-2.155715	-0.277891
N	0.690541	0.122972	2.407031
H	-0.288143	-0.153457	2.284641
H	0.765357	0.440024	3.375503
H	0.773841	0.967461	1.831743
N	4.078080	-0.006349	-0.432891
H	5.032088	0.190030	-0.125307
H	4.064096	0.203460	-1.433353
H	3.489914	0.712997	-0.002442

(IIIId)

La state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-1.005221	-1.318449	-0.652511
C	-2.396721	-1.568568	-0.319105

C	-3.201737	-0.552843	0.153736
C	-2.664501	0.738338	0.301343
C	-1.318057	1.061073	-0.064543
C	-0.794193	2.375248	0.124659
C	0.520751	2.661828	-0.337583
C	1.298594	1.682140	-0.925268
C	0.825292	0.338141	-1.043631
C	-0.501140	0.047645	-0.605280
O	-0.238161	-2.288783	-0.915552
H	-2.743798	-2.596967	-0.424644
H	-4.241828	-0.743497	0.420043
H	-3.296669	1.541443	0.686413
H	-1.425207	3.154899	0.549106
H	0.909283	3.678447	-0.249676
H	2.277669	1.952671	-1.332235
H	1.375175	-0.421690	-1.597736
N	1.781756	-1.936785	0.794964
H	1.347014	-1.213079	1.449317
H	2.654652	-1.499103	0.406648
H	1.992455	-2.800690	1.296418
H	1.078392	-2.118375	0.010522
N	0.606627	0.130554	2.301545
H	-0.407321	-0.013886	2.282641
H	0.828905	0.444667	3.247804
H	0.734906	0.946425	1.688173
N	3.902584	-0.312244	-0.208745
H	4.845755	-0.149738	0.148101
H	3.991412	-0.355515	-1.226670
H	3.369307	0.546255	-0.035067

(IIIe)

Ground state optimized

Atom	X	Y	Z
C	-1.356607	1.068661	-0.484025
C	-0.894075	2.348776	-0.299634
C	0.479742	2.639682	-0.397567

C	1.391283	1.654752	-0.661633
C	0.952329	0.325304	-0.866456
C	1.864337	-0.730417	-1.115920
C	1.425575	-2.011222	-1.302402
C	0.042804	-2.298410	-1.277226
C	-0.862744	-1.301898	-1.040067
C	-0.433688	0.025762	-0.804170
O	-2.674373	0.812626	-0.374508
H	-1.611149	3.122142	-0.063402
H	0.812529	3.658096	-0.246983
H	2.449188	1.875155	-0.726133
H	2.921857	-0.499004	-1.156520
H	2.134193	-2.806634	-1.490006
H	-0.296639	-3.309042	-1.458179
H	-1.922655	-1.512361	-1.038258
N	-2.909342	-1.128352	1.522273
H	-1.990153	-1.090621	1.972326
H	-3.098383	-2.096459	1.293102
H	-3.600456	-0.842687	2.205605
H	-2.820935	0.032668	0.234292
N	0.046803	-0.661568	2.241714
H	0.021175	0.292111	1.891984
H	0.760355	-0.674932	2.963052
H	0.413099	-1.216425	1.473188
N	3.124589	0.052733	2.135444
H	4.094502	0.345015	2.131898
H	3.052309	-0.739811	1.507495
H	2.588070	0.796155	1.701167

(IIIe)

Lb state optimized

Atom	X	Y	Z
C	-1.716432	0.744410	-0.117489
C	-1.737685	2.069233	0.371919
C	-0.557080	2.855719	0.359055
C	0.650420	2.309578	-0.091714

C	0.724415	0.984531	-0.588922
C	1.922370	0.405882	-1.060376
C	1.942139	-0.857936	-1.652851
C	0.715110	-1.567835	-1.846282
C	-0.486576	-1.028211	-1.385195
C	-0.521981	0.195442	-0.692235
O	-2.826233	0.028667	-0.024728
H	-2.669576	2.436999	0.798462
H	-0.583102	3.877033	0.737450
H	1.559680	2.915422	-0.079617
H	2.849646	0.977099	-0.964866
H	2.879860	-1.278972	-2.014828
H	0.717689	-2.522543	-2.371715
H	-1.423263	-1.558052	-1.564393
N	-2.240520	-2.366814	0.860711
H	-1.325426	-2.214033	1.326790
H	-2.132242	-3.196500	0.275231
H	-2.907508	-2.619179	1.592335
H	-2.611707	-0.962009	0.181104
N	0.428682	-1.435753	1.813093
H	0.174519	-0.444850	1.878375
H	1.199772	-1.544234	2.477453
H	0.884797	-1.498632	0.896939
N	3.266913	-0.337683	1.946022
H	4.163334	0.107565	2.153797
H	3.407338	-0.817130	1.052673
H	2.632327	0.429552	1.708387

(IIIe)

La state optimized

Atom	X	Y	Z
C	0.648371	1.550978	-0.562058
C	2.054059	1.695416	-0.224370
C	2.850053	0.583147	-0.049383
C	2.284016	-0.696932	-0.193595
C	0.913536	-0.901556	-0.555442

C	0.358571	-2.211919	-0.646061
C	-0.971992	-2.357048	-1.143279
C	-1.720000	-1.254089	-1.507684
C	-1.209939	0.067836	-1.344924
C	0.114490	0.225364	-0.837088
O	-0.098292	2.573041	-0.561896
H	2.419802	2.713470	-0.088343
H	3.905608	0.686559	0.204709
H	2.911040	-1.579134	-0.042809
H	0.989592	-3.082242	-0.464949
H	-1.390393	-3.357567	-1.268432
H	-2.718412	-1.396785	-1.927934
H	-1.737559	0.936112	-1.737306
N	-2.310296	1.999787	0.734296
H	-2.160458	0.984342	1.223771
H	-3.104185	1.928504	0.095947
H	-2.500448	2.732909	1.420694
H	-1.436166	2.255303	0.143932
N	-1.942945	-0.433847	1.763820
H	-1.029024	-0.573634	2.234478
H	-2.647770	-0.854357	2.372731
H	-1.895211	-1.025014	0.923227
N	0.795403	-1.164148	2.655525
H	1.206594	-1.617756	3.472387
H	0.766210	-1.871433	1.912082
H	1.485003	-0.483338	2.328804

(III_f)

Ground state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.028695	-0.744490	-0.000446
C	0.211944	-2.105408	0.000049
C	1.511468	-2.651213	0.000727
C	2.612396	-1.845725	0.000905
C	2.456828	-0.437749	0.000395
C	3.573114	0.432828	0.000539

C	3.407525	1.788789	0.000023
C	2.111573	2.345448	-0.000664
C	1.010016	1.535074	-0.000826
C	1.156799	0.128338	-0.000293
O	-1.196351	-0.177671	-0.001118
H	-0.651364	-2.756843	-0.000099
H	1.626225	-3.727128	0.001106
H	3.610046	-2.264391	0.001424
H	4.565359	-0.000919	0.001060
H	4.271113	2.440458	0.000140
H	1.988980	3.419966	-0.001065
H	0.019490	1.966978	-0.001342
H	-1.908180	-0.873097	-0.001262
N	-2.445419	2.679252	0.000420
H	-3.001175	2.864228	0.823750
H	-2.149925	1.708232	0.000787
H	-3.001402	2.863466	-0.822929
N	-3.319811	-1.920333	-0.001344
H	-4.108411	-1.269970	-0.000636
H	-3.405040	-2.515559	0.813594
H	-3.405616	-2.514542	-0.816963
N	-5.261803	0.503021	0.001422
H	-5.832724	0.694895	0.815586
H	-5.834195	0.696136	-0.811413
H	-4.505293	1.180532	0.001262

(III_f)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.000000	0.726456	0.000000
C	-0.181023	2.128242	0.000000
C	-1.487734	2.683685	0.000000
C	-2.605139	1.837849	0.000000
C	-2.467696	0.432568	0.000000
C	-3.577872	-0.443543	0.000000
C	-3.416494	-1.827303	0.000000

C	-2.107505	-2.394530	0.000000
C	-0.982422	-1.564638	0.000000
C	-1.113445	-0.164587	0.000000
O	1.226218	0.197178	0.000000
H	0.699171	2.770395	0.000000
H	-1.616520	3.765165	0.000000
H	-3.610471	2.264463	0.000000
H	-4.581120	-0.010931	0.000000
H	-4.292377	-2.476165	0.000000
H	-1.981573	-3.476602	0.000000
H	0.012688	-2.011698	0.000000
H	1.937521	0.921693	0.000000
N	2.463064	-2.653616	0.000000
H	3.050991	-2.789513	0.821588
H	2.149402	-1.679651	0.000000
H	3.050991	-2.789513	-0.821588
N	3.272899	1.916740	0.000000
H	4.069463	1.258108	0.000000
H	3.382578	2.520607	0.816280
H	3.382578	2.520607	-0.816280
N	5.161475	-0.454938	0.000000
H	5.739994	-0.677701	0.812181
H	5.739994	-0.677701	-0.812181
H	4.410843	-1.151484	0.000000

(III_f)

La state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-0.612748	-0.453093	-0.849442
C	-1.072996	-1.800557	-0.606356
C	-0.236656	-2.695461	0.009872
C	1.069003	-2.278518	0.398043
C	1.573558	-0.983325	0.127062
C	2.869815	-0.577316	0.514167
C	3.332131	0.735153	0.207009
C	2.520552	1.622201	-0.462555

C	1.196636	1.243971	-0.852209
C	0.725817	-0.046701	-0.550708
O	-1.443177	0.453535	-1.330564
H	-2.073557	-2.076132	-0.938515
H	-0.556345	-3.720347	0.195941
H	1.726313	-2.994365	0.896188
H	3.505793	-1.274977	1.059326
H	4.338257	1.030700	0.506727
H	2.880161	2.622676	-0.705834
H	0.562513	1.928475	-1.412773
H	-2.421425	0.195391	-1.093114
N	-1.100831	3.172038	0.509130
H	-0.172088	2.947152	0.871547
H	-1.321392	2.405611	-0.131378
H	-1.747159	3.090192	1.295238
N	-3.725316	-0.022107	-0.216403
H	-3.247118	-0.066559	0.702958
H	-4.328573	-0.841542	-0.297309
H	-4.343158	0.791203	-0.195821
N	-1.676649	0.143956	1.973299
H	-1.001009	-0.621954	1.892475
H	-1.730280	0.353237	2.972433
H	-1.196615	0.947627	1.554938

(IVa)

Ground state optimized

Atom	X	Y	Z
C	0.419357	-0.182230	-0.980692
C	0.959542	-1.410717	-0.676735
C	0.156361	-2.423193	-0.115063
C	-1.171348	-2.220425	0.137819
C	-1.756165	-0.963817	-0.152966
C	-3.117010	-0.689329	0.127238
C	-3.648702	0.547284	-0.110200
C	-2.845987	1.576084	-0.649628
C	-1.531795	1.339384	-0.945936

C	-0.958593	0.070285	-0.703816
O	1.121526	0.818388	-1.530562
H	2.005078	-1.597005	-0.878415
H	0.607345	-3.381892	0.106540
H	-1.786425	-3.004906	0.558243
H	-3.728282	-1.479723	0.544521
H	-4.688751	0.742263	0.114459
H	-3.276423	2.551306	-0.831445
H	-0.905970	2.114264	-1.364664
N	3.782450	0.379053	-1.391337
H	4.258209	1.272958	-1.361177
H	4.256752	-0.190541	-2.081208
H	3.896104	-0.059762	-0.470742
H	2.103987	0.605213	-1.552092
N	3.499733	-0.622823	1.451483
H	4.162424	-0.685855	2.214396
H	2.985609	0.257274	1.555143
H	2.824942	-1.367533	1.582033
N	1.790462	1.964740	1.297564
H	0.950576	1.652477	1.786200
H	1.996413	2.903241	1.616266
H	1.545201	2.024345	0.314403
N	-0.782083	0.588171	2.519356
H	-1.579077	0.893404	1.969612
H	-0.584451	-0.360555	2.217986
H	-1.083371	0.539984	3.484857

(IVa)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-0.490928	0.366375	-0.854439
C	-1.098402	1.481981	-0.226388
C	-0.308347	2.376410	0.540747
C	1.068067	2.163691	0.694247
C	1.713744	1.052809	0.101199
C	3.092991	0.792140	0.252245

C	3.693454	-0.327470	-0.322905
C	2.904290	-1.239126	-1.093759
C	1.540347	-1.007272	-1.276772
C	0.907400	0.109030	-0.700520
O	-1.183414	-0.482829	-1.596136
H	-2.166947	1.647349	-0.349329
H	-0.777194	3.242237	1.007953
H	1.664365	2.866481	1.280399
H	3.693192	1.491688	0.839143
H	4.760565	-0.504014	-0.192141
H	3.373587	-2.109567	-1.552055
H	0.937551	-1.693940	-1.871919
N	-3.759242	-0.022588	-1.488393
H	-4.317265	-0.809606	-1.823341
H	-4.135831	0.809115	-1.946232
H	-3.942284	0.071089	-0.466002
H	-2.195384	-0.256542	-1.598530
N	-3.720672	0.055971	1.432830
H	-4.444130	-0.227669	2.096481
H	-3.021601	-0.711843	1.422561
H	-3.241521	0.842582	1.876547
N	-1.636875	-2.104460	1.040081
H	-0.733709	-1.932927	1.507841
H	-1.833085	-3.096121	1.190329
H	-1.429356	-2.018574	0.041106
N	1.185915	-1.442237	2.164555
H	1.819511	-1.631526	1.382134
H	1.136562	-0.420273	2.194387
H	1.700707	-1.713513	3.004303

(IVa)

La state optimized

Atom	X	Y	Z
C	-0.591661	0.433684	-0.832482
C	-1.272545	1.467950	-0.091852
C	-0.550880	2.287790	0.739580

C	0.849793	2.098739	0.858939
C	1.553012	1.085227	0.160504
C	2.952169	0.900247	0.308949
C	3.608768	-0.119455	-0.439875
C	2.894439	-0.951922	-1.274130
C	1.475746	-0.813087	-1.408464
C	0.821759	0.219932	-0.704447
O	-1.251958	-0.357932	-1.636492
H	-2.348580	1.578707	-0.215865
H	-1.041683	3.081795	1.301830
H	1.418102	2.759459	1.517373
H	3.516381	1.569092	0.958706
H	4.690116	-0.235274	-0.351186
H	3.410590	-1.722470	-1.848964
H	0.906883	-1.448463	-2.082831
N	-3.815946	-0.158411	-1.395836
H	-4.285594	-0.995025	-1.745869
H	-4.313806	0.639173	-1.794703
H	-3.949279	-0.136434	-0.359276
H	-2.297686	-0.219724	-1.584742
N	-3.603791	-0.220425	1.499727
H	-4.251895	-0.681269	2.141779
H	-2.781562	-0.852306	1.421011
H	-3.261108	0.597779	2.008259
N	-1.251926	-2.052245	0.988805
H	-0.353677	-1.841235	1.453980
H	-1.427062	-3.035838	1.208789
H	-1.023856	-2.045659	-0.010161
N	1.642724	-1.693678	1.967265
H	1.985351	-1.824929	1.009407
H	1.994994	-0.762705	2.205891
H	2.188011	-2.342529	2.538441

(IVb)

Ground state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
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C	-0.270469	-0.168847	0.952404
C	-0.970257	1.012615	1.023516
C	-0.349341	2.229375	0.681259
C	0.953160	2.270993	0.269523
C	1.708618	1.074372	0.205631
C	3.065986	1.066022	-0.199187
C	3.781980	-0.096397	-0.238852
C	3.177841	-1.316922	0.132580
C	1.868155	-1.344816	0.524365
C	1.101769	-0.156594	0.558878
O	-0.811891	-1.366161	1.234378
H	-2.007647	0.999560	1.325833
H	-0.925771	3.143409	0.740709
H	1.424827	3.207275	0.002369
H	3.528442	2.005932	-0.473475
H	4.818468	-0.084482	-0.547991
H	3.758650	-2.229193	0.114121
H	1.396883	-2.270587	0.823286
H	-1.810660	-1.296446	1.325681
N	-3.510528	-1.222541	1.277370
H	-3.749063	-0.508784	0.576779
H	-3.961930	-0.968824	2.147963
H	-3.919229	-2.099512	0.977475
N	-3.872989	0.963176	-0.825751
H	-3.900776	1.915133	-0.478648
H	-3.003413	0.873734	-1.363585
H	-4.637484	0.880814	-1.485890
N	-1.168949	0.635539	-2.323213
H	-0.921325	-0.350780	-2.235238
H	-0.992900	0.903197	-3.284059
H	-0.509576	1.151680	-1.748834
N	-0.307185	-2.353205	-1.720738
H	0.704599	-2.362659	-1.773710
H	-0.544183	-2.328895	-0.732957
H	-0.639882	-3.230879	-2.099230

(IVb)

Lb state optimized

Atom	X	Y	Z
C	0.271520	-0.239955	-0.899807
C	1.024067	0.955823	-0.995267
C	0.404650	2.201868	-0.719547
C	-0.942080	2.261445	-0.333585
C	-1.731426	1.093149	-0.228715
C	-3.088133	1.111763	0.159147
C	-3.849713	-0.055027	0.216278
C	-3.256774	-1.306905	-0.136295
C	-1.917236	-1.366670	-0.522606
C	-1.115190	-0.209930	-0.556060
O	0.816832	-1.431198	-1.111177
H	2.080128	0.904087	-1.251469
H	0.986309	3.120187	-0.798573
H	-1.402873	3.227625	-0.116593
H	-3.542810	2.072357	0.412672
H	-4.895932	-0.011645	0.516786
H	-3.857825	-2.216073	-0.118508
H	-1.466692	-2.319151	-0.805580
H	1.840260	-1.362247	-1.253799
N	3.427227	-1.291904	-1.328675
H	3.743238	-0.586758	-0.627071
H	3.814195	-1.008114	-2.230653
H	3.883351	-2.174865	-1.092879
N	3.994229	0.786080	0.695649
H	4.081858	1.751261	0.368474
H	3.129972	0.777023	1.272841
H	4.764738	0.667669	1.357416
N	1.408264	0.725691	2.280564
H	1.034273	-0.235521	2.261415
H	1.320675	1.030554	3.252363
H	0.720607	1.280337	1.762741
N	0.123631	-2.080563	1.912185
H	-0.885756	-1.920312	1.868531

H	0.404010	-2.203398	0.934434
H	0.242040	-2.991924	2.357538

(IVb)

La state optimized

Atom	X	Y	Z
C	-0.279346	-0.171423	-0.915952
C	-1.067381	1.038104	-0.973496
C	-0.492013	2.234383	-0.626718
C	0.865378	2.258585	-0.206511
C	1.683844	1.099869	-0.175584
C	3.040168	1.142708	0.221696
C	3.825227	-0.045589	0.198259
C	3.278064	-1.239853	-0.213151
C	1.905721	-1.312469	-0.612777
C	1.113064	-0.148983	-0.574028
O	-0.822732	-1.336084	-1.183478
H	-2.108971	0.969407	-1.282728
H	-1.066321	3.159741	-0.661578
H	1.315100	3.212971	0.076316
H	3.473692	2.089947	0.541921
H	4.871331	-0.000712	0.504456
H	3.889865	-2.142685	-0.241379
H	1.471690	-2.245718	-0.965821
H	-1.870642	-1.280409	-1.294242
N	-3.405231	-1.252314	-1.304200
H	-3.713617	-0.546550	-0.595827
H	-3.805872	-2.150755	-1.028993
H	-3.845565	-1.005652	-2.192521
N	-3.908387	0.784384	0.742087
H	-4.674873	0.655102	1.406458
H	-3.036695	0.718810	1.307065
H	-3.970708	1.766494	0.463242
N	-1.332635	0.514374	2.290058
H	-1.002028	-0.462715	2.241226
H	-0.583800	1.053865	1.844588

H	-1.283824	0.765627	3.280039
N	-0.087601	-2.249601	1.783744
H	-0.138116	-3.173105	2.217308
H	-0.347321	-2.384855	0.802016
H	0.909164	-2.020025	1.734010

(IVc)

Ground state optimized

Atom	X	Y	Z
C	0.142330	0.135931	-0.230914
C	0.816006	-0.493159	0.791414
C	0.104247	-1.208251	1.777300
C	-1.257616	-1.305269	1.739209
C	-1.979680	-0.680174	0.693191
C	-3.391268	-0.753795	0.608155
C	-4.067793	-0.136373	-0.405563
C	-3.366334	0.590890	-1.390812
C	-2.003192	0.681404	-1.339428
C	-1.281052	0.048311	-0.301662
O	0.761328	0.846431	-1.190048
H	1.896076	-0.437845	0.830323
H	0.657839	-1.688707	2.573513
H	-1.798940	-1.856672	2.496567
H	-3.926327	-1.311459	1.366673
H	-5.146346	-0.202352	-0.455899
H	-3.912929	1.076830	-2.187533
H	-1.450430	1.232633	-2.086582
H	1.781747	-1.000902	-2.018075
N	2.187823	-1.907260	-1.803964
H	2.324974	-2.392063	-2.682346
H	1.474608	-2.413728	-1.291543
H	3.802082	-1.485033	-0.445025
N	4.434448	-1.089923	0.254335
H	5.379166	-1.203906	-0.092579
H	3.692769	0.895370	0.067065
H	4.362088	-1.664229	1.085463

N	3.094136	1.662589	-0.243225
H	2.726989	2.164957	0.563716
H	3.650635	2.305848	-0.791232
H	1.699943	1.115906	-0.890740
N	0.753322	2.816023	1.432488
H	0.313605	2.779697	0.518036
H	0.389461	2.018294	1.942502
H	0.410370	3.648814	1.895296

(IVc)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.151548	0.132894	-0.285866
C	0.863977	-0.650977	0.660199
C	0.155349	-1.484092	1.567187
C	-1.244727	-1.556155	1.520959
C	-1.992626	-0.808339	0.583981
C	-3.403759	-0.847388	0.515191
C	-4.111541	-0.079880	-0.406562
C	-3.410588	0.777598	-1.310044
C	-2.017855	0.847090	-1.270667
C	-1.275427	0.079148	-0.355336
O	0.781370	0.944113	-1.123649
H	1.953246	-0.610795	0.669742
H	0.706279	-2.080841	2.293721
H	-1.778128	-2.205377	2.218885
H	-3.940562	-1.497515	1.210225
H	-5.199525	-0.132339	-0.438165
H	-3.965846	1.375937	-2.031969
H	-1.473960	1.498019	-1.956100
H	1.988256	-0.680216	-2.074738
N	2.482261	-1.574659	-1.996727
H	2.648905	-1.881456	-2.957145
H	1.773094	-2.212295	-1.626179
H	3.939591	-1.222696	-0.564046
N	4.480847	-0.846662	0.231661

H	5.458447	-0.852346	-0.064556
H	3.582028	0.961289	0.267054
H	4.422588	-1.554898	0.965966
N	2.920848	1.718339	0.026367
H	2.458305	2.062222	0.880216
H	3.448739	2.491816	-0.377640
H	1.736140	1.230246	-0.723114
N	0.574022	2.428957	1.796911
H	0.009973	2.519022	0.946018
H	0.260007	1.542523	2.201973
H	0.229508	3.155581	2.427298

(IVc)

La state optimized

Atom	X	Y	Z
C	0.746787	-0.549728	-0.855335
C	1.396868	-1.659937	-0.174424
C	0.683250	-2.478428	0.677751
C	-0.688214	-2.239157	0.878552
C	-1.395157	-1.192439	0.206829
C	-2.786117	-0.968683	0.438233
C	-3.469298	-0.013819	-0.373798
C	-2.780890	0.765893	-1.282115
C	-1.366129	0.649484	-1.430411
C	-0.691835	-0.370853	-0.697892
O	1.424651	0.284918	-1.517494
H	2.466200	-1.794547	-0.346581
H	1.171106	-3.307094	1.192823
H	-1.249979	-2.885221	1.556651
H	-3.332231	-1.623368	1.116828
H	-4.551565	0.094607	-0.277260
H	-3.327904	1.474969	-1.908113
H	-0.825504	1.193535	-2.202664
H	3.400294	0.226931	-1.257353
N	4.301007	0.213674	-0.756396
H	4.845512	0.988838	-1.139267

H	4.783535	-0.628813	-1.074823
H	3.352761	0.491514	0.988076
N	2.643569	0.712447	1.711463
H	3.153234	0.955854	2.562518
H	1.514407	1.755681	0.985326
H	2.171248	-0.175181	1.905553
N	0.778952	2.291579	0.407307
H	-0.199981	2.198924	0.854860
H	1.036501	3.274419	0.319327
H	0.768659	1.849225	-0.531118
N	-1.735864	1.977563	1.528472
H	-2.430307	2.318957	0.857410
H	-1.928620	0.964412	1.532715
H	-2.023803	2.326175	2.444790

(IVd)

Ground state optimized

Atom	X	Y	Z
C	0.229942	0.937701	-0.391444
C	0.520941	2.264350	-0.192627
C	1.826615	2.660261	0.161263
C	2.825669	1.742794	0.313546
C	2.557591	0.367004	0.111868
C	3.561356	-0.620733	0.260888
C	3.282606	-1.943633	0.065697
C	1.980026	-2.350050	-0.294462
C	0.986983	-1.422589	-0.447920
C	1.250564	-0.047460	-0.245508
O	-1.002118	0.496731	-0.715898
H	-0.259651	3.002592	-0.316873
H	2.030253	3.712144	0.311451
H	3.826945	2.049255	0.585381
H	4.560094	-0.304100	0.534295
H	4.061251	-2.685153	0.183385
H	1.771718	-3.399276	-0.454481
H	-0.011139	-1.726627	-0.733784

N	-4.543101	-0.303249	0.673261
H	-5.484596	-0.376104	1.037832
H	-3.921722	-0.776584	1.324699
H	-4.490932	-0.861121	-0.176435
N	-3.067383	2.151366	-0.310671
H	-3.697557	1.433494	0.071620
H	-2.982020	2.890586	0.376268
H	-3.508707	2.551667	-1.129527
H	-1.701636	1.216561	-0.617941
N	-1.684753	-1.317707	1.783888
H	-0.910772	-1.972209	1.818656
H	-1.662069	-0.809002	2.660310
H	-1.452725	-0.649659	1.052135
N	-2.828723	-2.020552	-1.198468
H	-2.615582	-2.789485	-1.820713
H	-2.610912	-2.314049	-0.251065
H	-2.189340	-1.261644	-1.411896

(IVd)

Lb state optimized

Atom	X	Y	Z
C	0.185535	0.947113	-0.375003
C	0.483228	2.316087	-0.193329
C	1.807539	2.716356	0.125040
C	2.820088	1.758016	0.269559
C	2.563563	0.379068	0.099091
C	3.556001	-0.614432	0.251121
C	3.269298	-1.967809	0.077817
C	1.945101	-2.378413	-0.265451
C	0.935166	-1.426982	-0.426140
C	1.192927	-0.055037	-0.246544
O	-1.050775	0.536950	-0.653931
H	-0.312209	3.049931	-0.319225
H	2.035257	3.773654	0.254840
H	3.835288	2.074750	0.517419
H	4.569691	-0.301272	0.511386

H	4.056125	-2.711699	0.199256
H	1.725361	-3.435291	-0.414465
H	-0.074388	-1.741688	-0.698119
N	-4.464364	-0.311040	0.561947
H	-5.411493	-0.452253	0.916819
H	-3.839853	-0.791554	1.220739
H	-4.385993	-0.889000	-0.283437
N	-3.038283	2.142426	-0.212759
H	-3.688305	1.388778	0.102634
H	-2.963391	2.817897	0.549396
H	-3.488899	2.630198	-0.988299
H	-1.763997	1.285090	-0.538049
N	-1.710266	-1.377911	1.769859
H	-0.942389	-2.054469	1.766667
H	-1.620094	-0.895712	2.667087
H	-1.433959	-0.683613	1.066751
N	-2.712905	-2.037989	-1.223464
H	-2.340177	-2.779497	-1.817800
H	-2.501454	-2.311117	-0.259519
H	-2.118854	-1.220929	-1.388668

(IVd)

La state optimized

Atom	X	Y	Z
C	0.211992	0.945664	-0.294961
C	0.502653	2.349308	-0.138091
C	1.791851	2.738420	0.119444
C	2.810291	1.751336	0.232275
C	2.561790	0.365610	0.082077
C	3.583266	-0.604288	0.207018
C	3.277305	-1.984428	0.032838
C	1.991946	-2.386961	-0.249416
C	0.935255	-1.428694	-0.368230
C	1.226349	-0.059883	-0.201851
O	-1.023365	0.544766	-0.506240
H	-0.313207	3.064638	-0.242479

H	2.043909	3.791888	0.236869
H	3.833812	2.071705	0.438092
H	4.599629	-0.283687	0.434740
H	4.074040	-2.724014	0.122999
H	1.767848	-3.445321	-0.390014
H	-0.075679	-1.742739	-0.621821
N	-4.484386	-0.270186	0.447735
H	-5.445626	-0.402863	0.765771
H	-3.888380	-0.770933	1.119077
H	-4.380916	-0.833188	-0.405497
N	-3.006075	2.129430	-0.224033
H	-3.682255	1.376034	0.052794
H	-2.999629	2.826711	0.521958
H	-3.382716	2.591615	-1.053098
H	-1.762524	1.307371	-0.427409
N	-1.851164	-1.473929	1.790614
H	-1.161409	-2.230231	1.791604
H	-1.780281	-1.065253	2.725418
H	-1.438732	-0.775772	1.162288
N	-2.695529	-1.965240	-1.305723
H	-2.344588	-2.730092	-1.884005
H	-2.531250	-2.249697	-0.335630
H	-2.041240	-1.191331	-1.448520

(IVe)

Ground state optimized

Atom	X	Y	Z
C	0.162520	-0.756686	0.737734
C	-0.232259	-1.838385	-0.014399
C	0.568160	-2.295030	-1.081911
C	1.744986	-1.680083	-1.398490
C	2.182405	-0.565584	-0.641772
C	3.394515	0.107431	-0.931759
C	3.797679	1.181798	-0.190662
C	3.008525	1.640802	0.885857
C	1.832716	1.014519	1.192714

C	1.393166	-0.097437	0.437662
O	-0.560441	-0.256367	1.754090
H	-1.163243	-2.336920	0.217199
H	0.233452	-3.149971	-1.654575
H	2.355754	-2.032498	-2.218928
H	3.998820	-0.249744	-1.756222
H	4.726844	1.683676	-0.424988
H	3.340620	2.488503	1.469632
H	1.220626	1.349734	2.017858
H	-1.440740	-0.731906	1.849668
N	-3.024111	-1.356018	1.886644
H	-3.324296	-1.230877	0.911717
H	-3.649266	-0.822156	2.478095
H	-3.138634	-2.331021	2.135049
N	-3.339974	-0.735693	-1.058759
H	-3.712497	-1.359126	-1.764799
H	-3.774238	0.178708	-1.197933
H	-2.353196	-0.618833	-1.267012
N	-4.125395	2.276822	-1.305331
H	-3.170391	2.407068	-0.968324
H	-4.199020	2.744587	-2.200108
H	-4.742707	2.764830	-0.668567
N	-1.149907	2.188528	-0.207662
H	-0.728872	3.061679	0.088704
H	-1.142657	1.578252	0.605734
H	-0.491602	1.773410	-0.859006

(IVe)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.059473	-0.654662	0.802228
C	-0.422510	-1.815405	0.149470
C	0.363704	-2.448659	-0.849967
C	1.610614	-1.919928	-1.210230
C	2.127000	-0.759399	-0.591535
C	3.373337	-0.190196	-0.937925

C	3.858173	0.950619	-0.302350
C	3.093080	1.572615	0.731847
C	1.856360	1.041043	1.101361
C	1.334899	-0.101382	0.468422
O	-0.649930	-0.025607	1.730936
H	-1.392798	-2.219838	0.433272
H	-0.007480	-3.350095	-1.336382
H	2.205868	-2.410626	-1.983220
H	3.962543	-0.668052	-1.724130
H	4.824362	1.364821	-0.589362
H	3.480369	2.456281	1.238340
H	1.270525	1.505500	1.895406
H	-1.592325	-0.442946	1.846842
N	-3.095602	-0.938734	1.907577
H	-3.418775	-0.948312	0.914649
H	-3.713739	-0.306087	2.418261
H	-3.262880	-1.870017	2.292449
N	-3.584237	-0.807504	-0.982267
H	-4.271971	-1.317088	-1.540374
H	-3.700963	0.190622	-1.231665
H	-2.674516	-1.068515	-1.373313
N	-3.607092	2.184553	-1.615962
H	-2.698567	2.404537	-1.177149
H	-3.527957	2.503403	-2.583530
H	-4.281478	2.819778	-1.184935
N	-0.860803	2.466671	-0.211140
H	-0.409917	3.314065	0.140383
H	-0.948631	1.856543	0.607882
H	-0.132874	2.008104	-0.766285

(IVe)

La state optimized

Atom	X	Y	Z
C	-0.279341	0.171444	0.915948
C	-1.067379	-1.038080	0.973511
C	-0.492015	-2.234366	0.626749

C	0.865375	-2.258577	0.206540
C	1.683844	-1.099864	0.175598
C	3.040167	-1.142712	-0.221686
C	3.825231	0.045582	-0.198263
C	3.278074	1.239853	0.213136
C	1.905732	1.312478	0.612763
C	1.113070	0.148995	0.574025
O	-0.822725	1.336111	1.183456
H	-2.108968	-0.969375	1.282740
H	-1.066326	-3.159721	0.661623
H	1.315095	-3.212967	-0.076274
H	3.473687	-2.089956	-0.541900
H	4.871334	0.000697	-0.504460
H	3.889879	2.142683	0.241354
H	1.471703	2.245734	0.965795
H	-1.870634	1.280442	1.294217
N	-3.405225	1.252344	1.304185
H	-3.713621	0.546574	0.595822
H	-3.805884	2.150780	1.028986
H	-3.845539	1.005680	2.192516
N	-3.908409	-0.784376	-0.742065
H	-4.674894	-0.655096	-1.406437
H	-3.036717	-0.718831	-1.307046
H	-3.970746	-1.766479	-0.463197
N	-1.332661	-0.514429	-2.290048
H	-1.002036	0.462654	-2.241216
H	-0.583836	-1.053934	-1.844578
H	-1.283853	-0.765681	-3.280030
N	-0.087586	2.249541	-1.783788
H	-0.138092	3.173035	-2.217375
H	-0.347308	2.384827	-0.802064
H	0.909178	2.019963	-1.734040

(IVf)

Ground state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
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C	0.217353	0.048628	0.000000
C	1.591320	-0.044210	0.000000
C	2.221057	-1.306145	0.000000
C	1.492962	-2.461043	0.000000
C	0.077788	-2.401199	0.000000
C	-0.720403	-3.570813	0.000000
C	-2.084288	-3.492248	0.000000
C	-2.724776	-2.234960	0.000000
C	-1.983950	-1.086035	0.000000
C	-0.571629	-1.141633	0.000000
O	-0.434083	1.222922	0.000000
H	2.183378	0.861626	0.000000
H	3.302538	-1.348451	0.000000
H	1.979364	-3.427410	0.000000
H	-0.225284	-4.533844	0.000000
H	-2.679162	-4.395736	0.000000
H	-3.805141	-2.184822	0.000000
H	-2.460609	-0.116338	0.000000
H	0.221158	2.026587	0.000000
N	1.093893	3.329604	0.000000
H	1.663609	3.355093	0.839093
H	1.663609	3.355093	-0.839093
H	0.427351	4.095753	0.000000
N	1.492962	1.865656	2.695707
H	0.575838	1.657554	2.312011
H	2.010635	0.995405	2.649645
H	1.361149	2.077118	3.677528
N	-1.932956	4.029694	0.000000
H	-1.844300	3.017793	0.000000
H	-2.484862	4.277402	0.812057
H	-2.484862	4.277402	-0.812057
N	1.492962	1.865656	-2.695707
H	0.575838	1.657554	-2.312011
H	1.361149	2.077118	-3.677528
H	2.010635	0.995405	-2.649645

(IVf)

Lb state optimized

Atom	X	Y	Z
C	0.100376	-0.087450	0.467637
C	0.460087	-1.478756	0.463433
C	-0.527831	-2.484897	0.288393
C	-1.866492	-2.122694	0.075572
C	-2.278396	-0.768420	0.046424
C	-3.620704	-0.380325	-0.181035
C	-4.002386	0.952243	-0.190691
C	-3.024734	1.975472	0.037124
C	-1.696293	1.628222	0.258226
C	-1.279364	0.288916	0.268082
O	1.006038	0.816085	0.637446
H	1.499842	-1.741823	0.674762
H	-0.249729	-3.538501	0.329247
H	-2.621196	-2.900772	-0.063958
H	-4.365840	-1.162527	-0.349869
H	-5.044036	1.221502	-0.365800
H	-3.325908	3.023136	0.043726
H	-0.944530	2.399302	0.437122
H	2.276030	0.400097	-0.025649
N	3.239134	0.208106	-0.519369
H	3.833540	-0.154745	0.238648
H	3.081389	-0.476955	-1.291922
H	3.521462	1.142510	-0.854669
N	3.350123	-0.472417	2.284138
H	2.452744	0.009074	2.140041
H	3.094435	-1.372293	2.696700
H	3.816499	0.037960	3.036833
N	2.552462	2.976950	-0.876296
H	1.762186	2.569156	-0.359600
H	2.844491	3.789452	-0.330088
H	2.145734	3.365235	-1.729513
N	2.144935	-1.656338	-2.424521
H	1.296982	-1.738059	-1.849072

H	1.828575	-1.312962	-3.333895
H	2.456855	-2.615436	-2.589280

(IVf)

La state optimized

Atom	X	Y	Z
C	-0.865385	-1.143488	-0.806001
C	-0.901054	-2.511402	-0.306083
C	0.212681	-3.082524	0.277705
C	1.397339	-2.339145	0.378608
C	1.514795	-1.006322	-0.141463
C	2.729050	-0.268056	-0.000377
C	2.837576	0.992779	-0.657066
C	1.760157	1.546602	-1.317014
C	0.491982	0.885148	-1.349043
C	0.412253	-0.436811	-0.797114
O	-1.926357	-0.577435	-1.168083
H	-1.849588	-3.043210	-0.402355
H	0.178667	-4.104026	0.659096
H	2.273575	-2.785322	0.853157
H	3.593702	-0.735073	0.470403
H	3.792092	1.523859	-0.641780
H	1.877633	2.502362	-1.832859
H	-0.306664	1.225640	-2.008092
H	-0.546399	1.344466	0.234263
N	-1.060642	1.637038	1.108856
H	-1.568802	0.802130	1.496345
H	-0.310112	2.002255	1.738402
H	-1.767823	2.307965	0.763851
N	-2.624691	-0.676535	1.747628
H	-2.912582	-0.797974	0.769633
H	-2.085808	-1.518301	1.965367
H	-3.468770	-0.718695	2.320034
N	-2.927635	2.333045	-0.898708
H	-2.655058	1.379090	-1.176862
H	-3.946267	2.361256	-0.970937

H	-2.592220	2.934511	-1.654319
N	1.522092	2.113628	2.143858
H	1.954428	2.777190	1.495175
H	1.963632	2.281430	3.049414
H	1.886973	1.208998	1.812386

(IVg)

Ground state optimized

Atom	X	Y	Z
C	-0.099916	-0.092388	-0.000055
C	0.092323	-1.456470	0.000140
C	-1.012417	-2.333572	0.000291
C	-2.293700	-1.862029	0.000246
C	-2.528276	-0.465035	0.000047
C	-3.837576	0.074279	-0.000003
C	-4.042298	1.425116	-0.000191
C	-2.944318	2.311288	-0.000338
C	-1.666933	1.823770	-0.000294
C	-1.430306	0.430332	-0.000102
O	0.902260	0.798102	-0.000214
H	1.098581	-1.852785	0.000182
H	-0.829028	-3.400327	0.000449
H	-3.137871	-2.538725	0.000360
H	-4.677599	-0.609156	0.000110
H	-5.049317	1.820431	-0.000227
H	-3.118050	3.378799	-0.000485
H	-0.814666	2.487817	-0.000406
H	1.825230	0.351168	-0.000081
N	3.267774	-0.374938	0.000145
H	4.106420	0.203138	0.000090
H	3.262859	-0.955697	-0.833711
H	3.262753	-0.955367	0.834232
N	1.822471	-0.967985	2.697950
H	1.494199	-0.091026	2.304233
H	1.028985	-1.597457	2.659759
H	2.018003	-0.798065	3.677135

N	1.822772	-0.969142	-2.697548
H	1.494166	-0.092243	-2.303978
H	1.029424	-1.598802	-2.659614
H	2.018605	-0.799217	-3.676673
N	5.722434	1.685363	-0.000171
H	6.681507	1.360900	-0.000367
H	5.610216	2.278534	0.812972
H	5.609846	2.278423	-0.813345

(IVg)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-0.091137	-0.056589	-0.000184
C	0.142076	-1.459395	0.000219
C	-0.952229	-2.365849	0.000597
C	-2.269511	-1.884921	0.000549
C	-2.550504	-0.500269	0.000139
C	-3.865955	0.018700	0.000082
C	-4.110317	1.388479	-0.000327
C	-3.017119	2.309626	-0.000697
C	-1.705301	1.835206	-0.000648
C	-1.427486	0.458434	-0.000243
O	0.899868	0.815407	-0.000524
H	1.167474	-1.827357	0.000273
H	-0.763310	-3.439087	0.000911
H	-3.104560	-2.589148	0.000834
H	-4.702351	-0.684633	0.000367
H	-5.135352	1.758846	-0.000363
H	-3.209856	3.382162	-0.001019
H	-0.863877	2.528897	-0.000926
H	1.884183	0.359359	-0.000225
N	3.204698	-0.269537	0.000240
H	4.027577	0.349404	0.000141
H	3.227772	-0.855187	-0.841601
H	3.227447	-0.854483	0.842582
N	1.954049	-1.010248	2.643256

H	1.501034	-0.156111	2.303337
H	1.202181	-1.703593	2.632131
H	2.147549	-0.837491	3.632055
N	1.954871	-1.012520	-2.642573
H	1.501524	-0.158346	-2.303188
H	1.203143	-1.706016	-2.631545
H	2.148805	-0.840099	-3.631346
N	5.580750	1.743820	-0.000142
H	6.545006	1.406400	-0.000563
H	5.510812	2.360930	0.811351
H	5.510183	2.361158	-0.811406

(IVg)

La state optimized

Atom	X	Y	Z
C	0.641488	-1.215295	0.877669
C	0.680807	-2.576275	0.366827
C	-0.398436	-3.110393	-0.308741
C	-1.545319	-2.321397	-0.507333
C	-1.655119	-0.981798	-0.011853
C	-2.794531	-0.175319	-0.310949
C	-2.891139	1.118183	0.277387
C	-1.877372	1.614147	1.073736
C	-0.679374	0.866168	1.292796
C	-0.591965	-0.446543	0.741157
O	1.677730	-0.683639	1.361286
H	1.602584	-3.135889	0.532759
H	-0.367810	-4.131967	-0.689544
H	-2.395464	-2.738217	-1.051924
H	-3.617477	-0.594104	-0.889368
H	-3.792263	1.713443	0.116213
H	-2.002606	2.586280	1.559278
H	0.086506	1.200114	1.991538
H	1.586512	0.956880	0.322733
N	1.842184	1.401492	-0.579177
H	1.589390	2.412193	-0.523930

H	1.214459	0.960335	-1.312929
H	2.843630	1.165820	-0.720979
N	4.227123	-0.105614	-0.151217
H	3.566586	-0.575562	0.483921
H	4.595275	-0.836379	-0.762737
H	5.015736	0.178501	0.432721
N	-0.055937	0.258227	-2.349584
H	-0.965132	0.499129	-1.931431
H	-0.016583	-0.761063	-2.255716
H	-0.139062	0.447628	-3.349995
N	0.334817	3.800677	-0.254589
H	0.114874	4.556521	-0.905687
H	0.393121	4.241430	0.666229
H	-0.505662	3.211672	-0.203642

(IVh)

Ground state optimized

Atom	X	Y	Z
C	0.728820	-0.585225	-1.172376
C	1.115369	-1.910542	-0.876494
C	0.296544	-2.771593	-0.141627
C	-0.929838	-2.378328	0.353553
C	-1.420388	-1.090404	0.018570
C	-2.701408	-0.641158	0.431459
C	-3.185827	0.579093	0.043152
C	-2.414327	1.420740	-0.786120
C	-1.158974	1.025775	-1.169876
C	-0.625353	-0.214170	-0.765575
O	1.500481	0.262389	-1.722218
H	2.081989	-2.242695	-1.232798
H	0.649412	-3.776045	0.063280
H	-1.549103	-3.055149	0.926275
H	-3.306520	-1.298509	1.044178
H	-4.173931	0.891533	0.355220
H	-2.818617	2.367160	-1.118815
H	-0.550020	1.641837	-1.817378

H	2.929254	0.140882	-0.516149
N	3.436887	0.041729	0.376549
H	3.968810	0.890910	0.524820
H	4.106068	-0.710263	0.261952
H	2.087672	-0.295678	1.437015
N	1.210918	-0.492526	2.010672
H	1.465186	-0.791328	2.945773
H	0.594118	0.395340	2.058558
H	0.677966	-1.240800	1.551690
N	-0.317757	1.779445	1.950693
H	0.222810	2.305524	1.254241
H	-1.211618	1.552099	1.523235
H	-0.496645	2.380930	2.744935
N	1.435367	2.863883	-0.315028
H	2.368758	3.255260	-0.269487
H	1.485757	2.009991	-0.883810
H	0.879182	3.527043	-0.843190

(IVh)

Lb state optimized

Atom	X	Y	Z
C	0.781261	-0.526538	-1.187871
C	1.308508	-1.826349	-0.875193
C	0.518884	-2.781861	-0.183710
C	-0.765337	-2.452858	0.269660
C	-1.339891	-1.168328	0.029750
C	-2.625969	-0.805368	0.482262
C	-3.212910	0.402952	0.125483
C	-2.521224	1.281520	-0.784277
C	-1.245646	0.958574	-1.220816
C	-0.591801	-0.209195	-0.791313
O	1.505949	0.351924	-1.743237
H	2.319514	-2.055142	-1.215063
H	0.910202	-3.784346	-0.003279
H	-1.362078	-3.202288	0.796716
H	-3.175034	-1.511422	1.112529

H	-4.213006	0.653981	0.478187
H	-3.011827	2.187527	-1.141822
H	-0.720266	1.606185	-1.926576
H	3.024222	0.375395	-0.500471
N	3.494484	0.330289	0.417088
H	3.995479	1.213816	0.531402
H	4.215713	-0.387096	0.319572
H	2.135478	-0.108822	1.465057
N	1.275224	-0.400176	2.021912
H	1.553618	-0.662126	2.968298
H	0.509688	0.437165	2.043104
H	0.868226	-1.222574	1.556983
N	-0.460169	1.607403	1.930269
H	0.001763	2.220505	1.231738
H	-1.345136	1.306708	1.506498
H	-0.697120	2.181042	2.740947
N	1.056544	2.968381	-0.264811
H	1.922886	3.509820	-0.281779
H	1.232358	2.130983	-0.840151
H	0.389898	3.518728	-0.811052

(IVh)

La state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.729458	-0.421276	-1.254655
C	1.367292	-1.700137	-0.967354
C	0.718247	-2.667631	-0.225491
C	-0.566839	-2.400006	0.279478
C	-1.263925	-1.179067	0.001100
C	-2.546257	-0.910792	0.570213
C	-3.268746	0.243133	0.121871
C	-2.691262	1.137557	-0.757887
C	-1.360795	0.953331	-1.228180
C	-0.655798	-0.224453	-0.838581
O	1.381301	0.502363	-1.806219
H	2.371617	-1.848757	-1.367894

H	1.194022	-3.628358	-0.022836
H	-1.075416	-3.155081	0.882948
H	-3.018934	-1.654849	1.210506
H	-4.286671	0.410783	0.478234
H	-3.264768	2.002386	-1.099018
H	-0.908479	1.623456	-1.955824
H	3.058270	0.609041	-0.712277
N	3.635957	0.586870	0.139840
H	4.181591	1.450811	0.129345
H	4.320766	-0.155398	-0.019734
H	2.300435	0.031417	1.563749
N	1.568379	-0.338185	2.198732
H	2.028456	-0.522762	3.092193
H	0.201063	0.624734	2.119926
H	1.320139	-1.253861	1.813488
N	-0.614141	1.297866	1.886546
H	-0.215159	1.968066	1.155425
H	-1.409974	0.753550	1.504766
H	-0.917891	1.810071	2.714226
N	0.762715	2.867038	0.015500
H	1.626066	3.357693	0.259032
H	1.014456	2.144726	-0.676758
H	0.191373	3.534361	-0.507160

(Va)

Ground state optimized

Atom	X	Y	Z
C	0.067746	0.670440	-0.959285
C	-0.144716	1.941040	-0.470425
C	0.856507	2.598932	0.272387
C	2.061702	2.005275	0.523236
C	2.314127	0.699024	0.037248
C	3.531186	0.025512	0.304059
C	3.736035	-1.254987	-0.128530
C	2.734914	-1.927442	-0.862472
C	1.553240	-1.300534	-1.147451

C	1.314056	0.019154	-0.701837
O	-0.839180	-0.006729	-1.670873
H	-1.083725	2.436828	-0.673490
H	0.660603	3.598429	0.638414
H	2.830078	2.517124	1.087091
H	4.296564	0.544917	0.867025
H	4.669518	-1.756994	0.087815
H	2.908491	-2.939342	-1.201945
H	0.780641	-1.799931	-1.714058
N	-3.286529	0.972701	-1.340361
H	-3.933552	0.183546	-1.317124
H	-3.667028	1.685777	-1.949698
H	-3.282090	1.321203	-0.381373
H	-1.759033	0.427948	-1.618881
N	-2.590287	0.841550	1.649600
H	-2.894832	0.894819	2.614196
H	-2.400018	-0.139889	1.450075
H	-1.692895	1.312422	1.597980
N	-1.671804	-2.051484	0.523921
H	-0.909813	-1.801907	1.156264
H	-1.677241	-3.061031	0.442396
H	-1.420454	-1.676314	-0.386728
N	0.650271	-0.856729	2.317965
H	1.495716	-1.226826	1.894455
H	0.660045	0.139812	2.124362
H	0.741380	-0.968546	3.320411
N	-4.747433	-1.241042	0.102707
H	-5.423727	-1.989521	0.184904
H	-4.979411	-0.548112	0.805521
H	-3.834078	-1.614043	0.360957

(Va)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.114765	0.463779	-1.003223
C	0.011177	1.867689	-0.810713

C	1.123041	2.597161	-0.317002
C	2.322185	1.944736	0.006633
C	2.461302	0.542947	-0.131393
C	3.628574	-0.155908	0.244541
C	3.718762	-1.542114	0.135447
C	2.608960	-2.286287	-0.377461
C	1.442767	-1.630320	-0.767979
C	1.319331	-0.232511	-0.658451
O	-0.882054	-0.244427	-1.487492
H	-0.912379	2.374440	-1.084647
H	1.048670	3.678557	-0.203100
H	3.171211	2.522850	0.378652
H	4.474224	0.416835	0.633440
H	4.632304	-2.056773	0.431156
H	2.682047	-3.369355	-0.476138
H	0.599298	-2.193354	-1.169740
N	-3.130345	0.894968	-1.272815
H	-3.832984	0.142746	-1.164688
H	-3.491145	1.586300	-1.930105
H	-3.065975	1.324012	-0.332367
H	-1.824875	0.301776	-1.495629
N	-2.702852	1.239535	1.629823
H	-3.020582	1.849589	2.385072
H	-3.129585	0.326268	1.811459
H	-1.705066	1.072796	1.807519
N	-1.890713	-1.726806	1.050957
H	-1.330134	-1.157383	1.695231
H	-1.551169	-2.683208	1.175661
H	-1.547871	-1.444134	0.125538
N	0.332445	0.241707	2.360149
H	0.904605	-0.497806	1.940735
H	0.676361	1.091841	1.902369
H	0.647638	0.310871	3.330179
N	-4.697660	-1.462659	-0.285118
H	-4.853551	-2.317239	-0.822921
H	-5.506089	-1.386509	0.334607

H -3.889835 -1.659959 0.324283

(Va)

La state optimized

Atom	X	Y	Z
C	-0.006098	0.970550	-1.113780
C	0.010611	2.357014	-0.667865
C	1.026800	2.830390	0.135142
C	2.056793	1.949456	0.524760
C	2.127628	0.594935	0.077352
C	3.191896	-0.263367	0.479678
C	3.293047	-1.555982	-0.114260
C	2.329990	-2.010445	-0.990981
C	1.189317	-1.211238	-1.311807
C	1.119872	0.107901	-0.789669
O	-1.015529	0.519866	-1.734272
H	-0.802276	2.999299	-1.013768
H	1.044835	3.870279	0.463607
H	2.859784	2.319384	1.166386
H	3.972910	0.117292	1.137541
H	4.149718	-2.189164	0.124428
H	2.437372	-2.996391	-1.448263
H	0.453540	-1.530533	-2.046638
N	-2.998931	1.111192	-0.007332
H	-3.799649	0.410354	0.000704
H	-3.357208	2.066305	-0.003659
H	-2.345521	0.960096	0.839279
H	-2.386158	0.960624	-0.855171
N	-1.132253	0.751847	2.028746
H	-1.390311	0.909548	3.005647
H	-0.647361	-0.165213	2.015604
H	-0.390884	1.430505	1.826493
N	-2.017127	-1.949652	-0.135536
H	-1.474397	-1.840961	0.727463
H	-1.750746	-2.874408	-0.483050
H	-1.560227	-1.300471	-0.791348

N	0.560643	-1.756635	1.900902
H	0.654261	-2.077138	0.929387
H	1.444240	-1.246536	2.031033
H	0.650851	-2.597045	2.475791
N	-4.831372	-0.997007	-0.006340
H	-5.384268	-1.237158	-0.830480
H	-5.381810	-1.294025	0.800404
H	-3.978313	-1.587072	-0.031721

(Vb)

Ground state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.205279	-0.385860	-0.195800
C	0.846882	-0.055987	0.977669
C	0.100158	0.287403	2.122989
C	-1.266844	0.318766	2.101283
C	-1.956601	0.013930	0.901934
C	-3.368641	0.073440	0.813239
C	-4.011625	-0.198481	-0.361436
C	-3.274233	-0.551310	-1.512074
C	-1.909609	-0.624824	-1.459336
C	-1.221642	-0.340437	-0.257233
O	0.850681	-0.758632	-1.309456
H	1.927782	-0.057007	1.013197
H	0.630134	0.532778	3.034246
H	-1.833837	0.582434	2.984216
H	-3.930944	0.344816	1.697939
H	-5.090775	-0.144787	-0.413201
H	-3.794005	-0.765380	-2.435972
H	-1.329367	-0.892676	-2.330578
N	3.349339	-1.399172	-0.718391
H	3.972859	-1.701756	-1.455555
H	3.140671	-2.200108	-0.124555
H	3.819353	-0.676737	-0.168586
H	1.838392	-0.943341	-1.119272
N	4.196862	1.209745	0.700190

H	5.112718	1.592877	0.499086
H	3.530403	1.660129	0.064593
H	3.963592	1.505181	1.640585
N	2.096596	2.161655	-1.387338
H	1.238454	2.573795	-1.019730
H	2.413386	2.760692	-2.140403
H	1.816456	1.282340	-1.810446
N	-0.766137	2.958598	-0.238535
H	-1.443077	2.462115	-0.807532
H	-0.683835	2.426456	0.622489
H	-1.177635	3.852145	0.001496
N	1.320848	-3.368517	0.540176
H	1.112264	-4.346002	0.702072
H	0.834729	-3.093572	-0.307665
H	0.885529	-2.841335	1.289108

(Vb)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-0.180733	0.326365	-0.235544
C	-0.873837	-0.075114	0.938920
C	-0.140098	-0.502640	2.075914
C	1.262435	-0.547071	2.051998
C	1.993074	-0.184293	0.896247
C	3.402188	-0.231773	0.827733
C	4.091388	0.137372	-0.325625
C	3.364922	0.587218	-1.472756
C	1.973479	0.653660	-1.443283
C	1.249039	0.274621	-0.295975
O	-0.822566	0.767049	-1.301194
H	-1.962856	-0.083064	0.939637
H	-0.674227	-0.802159	2.977727
H	1.810611	-0.873041	2.939004
H	3.954075	-0.566890	1.709379
H	5.179377	0.088715	-0.352398
H	3.903054	0.879172	-2.374560

H	1.414990	0.996630	-2.314975
N	-3.120520	1.615407	-0.615506
H	-3.707024	2.058508	-1.322556
H	-2.783765	2.349454	0.022703
H	-3.697260	0.933518	-0.091281
H	-1.836615	1.054379	-1.059250
N	-4.370391	-0.799172	0.620821
H	-5.333871	-1.047146	0.388777
H	-3.769342	-1.365083	-0.007178
H	-4.220912	-1.173065	1.560073
N	-2.399850	-2.006640	-1.339555
H	-1.559669	-2.479232	-0.973451
H	-2.696029	-2.570114	-2.139830
H	-2.024900	-1.145713	-1.749044
N	0.426534	-2.948194	-0.405878
H	1.000046	-2.262642	-0.906304
H	0.473006	-2.639049	0.568965
H	0.955888	-3.821412	-0.441323
N	-0.966699	3.258386	0.694989
H	-0.676812	4.191143	0.994515
H	-0.414545	3.057345	-0.144212
H	-0.587361	2.614774	1.395264

(Vb)

La state optimized

Atom	X	Y	Z
C	-0.660597	-0.561003	-0.394886
C	-1.364720	-1.081413	0.767671
C	-0.660306	-1.548233	1.859758
C	0.746641	-1.529588	1.837517
C	1.494956	-1.076308	0.706813
C	2.922873	-1.078361	0.708335
C	3.608826	-0.773894	-0.505581
C	2.916896	-0.358781	-1.626008
C	1.496380	-0.217088	-1.603037
C	0.795058	-0.625877	-0.432899

O	-1.298054	-0.008476	-1.340031
H	-2.455797	-1.054962	0.743910
H	-1.184687	-1.930611	2.736677
H	1.299933	-1.896981	2.704746
H	3.460285	-1.456900	1.577481
H	4.695329	-0.875434	-0.546080
H	3.460994	-0.148663	-2.549857
H	0.931925	0.029473	-2.500253
N	-0.024368	2.469402	-0.503647
H	-0.203271	3.361108	-0.965279
H	1.012685	2.399022	-0.209734
H	-0.656854	2.360719	0.370205
H	-0.250860	1.694025	-1.151714
N	-1.647795	2.011724	1.678864
H	-1.866117	2.707309	2.394172
H	-2.549777	1.699835	1.269133
H	-1.274267	1.196627	2.172917
N	-3.861835	1.098058	-0.085120
H	-4.350819	0.195948	-0.098268
H	-4.491788	1.758827	-0.544180
H	-3.092992	0.930259	-0.746848
N	-3.893656	-1.777795	-1.204629
H	-3.054106	-1.283365	-1.530677
H	-3.556124	-2.701606	-0.924912
H	-4.452979	-1.946304	-2.043199
N	2.604454	2.194081	0.319506
H	3.103569	2.850875	0.922370
H	3.203566	2.034397	-0.495447
H	2.642939	1.279195	0.794189

(Vc)

Ground state optimized

Atom	X	Y	Z
C	0.125892	-0.731814	-1.144543
C	0.340519	-2.042175	-0.783221
C	-0.629292	-2.746411	-0.041742

C	-1.791326	-2.146714	0.354976
C	-2.042509	-0.796427	0.002751
C	-3.230825	-0.130510	0.389857
C	-3.462543	1.165378	0.021734
C	-2.515844	1.864929	-0.757152
C	-1.353576	1.253892	-1.139885
C	-1.087995	-0.082205	-0.763583
O	1.002886	-0.020829	-1.866197
H	1.251129	-2.533811	-1.097377
H	-0.439594	-3.780364	0.215815
H	-2.535082	-2.690731	0.922201
H	-3.958765	-0.672641	0.980280
H	-4.377054	1.658435	0.322899
H	-2.711299	2.888416	-1.046281
H	-0.615323	1.782559	-1.724707
N	3.530703	-0.767894	-1.370660
H	4.145248	-0.143666	-1.880537
H	3.907160	-1.702509	-1.468940
H	3.582294	-0.495296	-0.381728
H	1.928271	-0.406174	-1.780101
N	3.411206	0.549251	1.370768
H	4.210954	0.720864	1.967787
H	3.233346	1.400814	0.834188
H	2.603537	0.439724	1.976478
N	2.011652	2.606604	-0.405405
H	1.314754	2.551266	0.339302
H	1.988159	3.543996	-0.785808
H	1.696998	1.970623	-1.130884
N	-0.039914	1.856053	1.920765
H	-0.933913	1.778530	1.447009
H	0.233641	0.914185	2.195633
H	-0.198425	2.382527	2.771205
N	0.912175	-1.166767	2.494517
H	1.140964	-1.630660	3.365132
H	1.593486	-1.462107	1.803389
H	0.020660	-1.535725	2.179575

(Vc)

Lb state optimized

Atom	X	Y	Z
C	-0.191486	1.002085	-0.825875
C	-0.227836	2.315449	-0.286919
C	0.926499	2.856288	0.337240
C	2.095748	2.091861	0.454684
C	2.166397	0.766786	-0.036974
C	3.320042	-0.039360	0.088017
C	3.348627	-1.352002	-0.377530
C	2.182540	-1.913895	-0.986723
C	1.027479	-1.145323	-1.139788
C	0.978236	0.188555	-0.698378
O	-1.226814	0.495971	-1.466064
H	-1.124479	2.917276	-0.425953
H	0.906152	3.878144	0.715108
H	2.978174	2.521301	0.934258
H	4.205338	0.390508	0.563161
H	4.254034	-1.949299	-0.275514
H	2.200591	-2.941889	-1.349919
H	0.132679	-1.581876	-1.586359
N	-3.477309	1.561354	-0.783706
H	-4.255025	1.162909	-1.313050
H	-3.689094	2.550977	-0.653373
H	-3.486272	1.092707	0.149894
H	-2.099257	1.042775	-1.285765
N	-3.112628	-0.236466	1.447475
H	-3.678636	-0.500683	2.255423
H	-3.188501	-1.018076	0.779171
H	-2.140220	-0.259812	1.773684
N	-2.697412	-2.190993	-0.876658
H	-1.961388	-2.593667	-0.277034
H	-2.962149	-2.921183	-1.538957
H	-2.220847	-1.469596	-1.423298
N	-0.478657	-2.857360	1.175773

H	0.464347	-2.986607	0.800478
H	-0.456943	-1.929214	1.615406
H	-0.564761	-3.524005	1.945380
N	0.025849	0.071206	2.421014
H	0.118469	0.302034	3.412532
H	-0.165528	0.961704	1.951392
H	0.971449	-0.169039	2.108045

(Vc)

La state optimized

Atom	X	Y	Z
C	-1.022839	0.807605	-1.279671
C	-1.090653	2.206598	-0.877530
C	0.018188	2.856214	-0.372466
C	1.226242	2.146706	-0.239428
C	1.371648	0.780787	-0.647436
C	2.615991	0.096856	-0.505509
C	2.731574	-1.228008	-1.024725
C	1.649627	-1.858620	-1.606110
C	0.377953	-1.218312	-1.689585
C	0.260336	0.117153	-1.209482
O	-2.065784	0.201751	-1.643677
H	-2.052305	2.707904	-1.002545
H	-0.034093	3.905203	-0.078275
H	2.106051	2.659049	0.158472
H	3.492233	0.637876	-0.145791
H	3.693778	-1.741071	-0.974618
H	1.770076	-2.863328	-2.017378
H	-0.448515	-1.654352	-2.247384
N	-3.459535	-0.110764	0.642469
H	-3.124293	-1.149945	0.580750
H	-4.415883	0.010509	0.969458
H	-2.727571	0.329297	1.288975
H	-3.303171	0.260278	-0.316592
N	-1.197261	0.560382	2.074422
H	-1.052888	0.889048	3.031375

H	-0.740711	-0.361865	2.045501
H	-0.590838	1.149533	1.494719
N	-2.111798	-2.408472	0.328380
H	-1.321749	-2.414905	0.992790
H	-2.396924	-3.378923	0.188781
H	-1.674298	-2.103888	-0.551964
N	0.604103	-2.000854	1.765968
H	1.005957	-1.845064	0.832338
H	1.068530	-1.305265	2.362757
H	0.971679	-2.907467	2.061267
N	1.977041	0.624752	2.792964
H	2.804888	0.678011	3.390425
H	1.644712	1.588467	2.714012
H	2.335348	0.399705	1.854563

(Vd)

Ground state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.632259	0.266643	-1.102918
C	0.378108	1.618950	-1.126222
C	1.253982	2.522822	-0.490940
C	2.374315	2.085622	0.156332
C	2.678933	0.702822	0.180142
C	3.835498	0.202148	0.826513
C	4.113315	-1.135304	0.836541
C	3.247885	-2.046871	0.194295
C	2.122521	-1.597068	-0.439170
C	1.809573	-0.217889	-0.455960
O	-0.182856	-0.640421	-1.664202
H	-0.499430	1.982860	-1.642735
H	1.027567	3.580614	-0.525575
H	3.044908	2.781380	0.642816
H	4.500091	0.905006	1.313226
H	5.001897	-1.500592	1.333641
H	3.482599	-3.102646	0.199713
H	1.455666	-2.281542	-0.944423

N	-2.665022	0.283488	-1.418605
H	-3.328489	-0.483920	-1.280905
H	-3.062733	0.914018	-2.104221
H	-2.615738	0.781952	-0.531092
H	-1.126796	-0.271074	-1.708431
N	-4.950443	0.840945	1.310634
H	-3.959587	1.079658	1.354378
H	-5.419105	1.604895	0.838754
H	-5.298847	0.831851	2.261606
N	-1.770683	1.242592	1.528931
H	-1.493449	0.257783	1.553520
H	-1.002093	1.734749	1.083959
H	-1.798927	1.567422	2.488683
N	-4.757136	-1.765641	-0.444624
H	-5.615823	-2.028291	-0.911909
H	-4.455062	-2.571958	0.087619
H	-4.978209	-1.022235	0.219764
N	-0.856858	-1.733057	1.170131
H	-0.803964	-1.713497	0.155278
H	0.096078	-1.845105	1.498088
H	-1.365051	-2.567489	1.434918

(Vd)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.498385	0.937459	-1.088145
C	0.534841	2.279728	-0.581794
C	1.514255	2.669939	0.365573
C	2.439849	1.737912	0.856580
C	2.459824	0.392247	0.401898
C	3.367940	-0.570388	0.891022
C	3.411276	-1.862147	0.381420
C	2.536151	-2.223544	-0.698137
C	1.622594	-1.302279	-1.193094
C	1.508810	-0.010941	-0.645937
O	-0.455231	0.552482	-1.852747

H	-0.176347	2.999346	-0.991347
H	1.554430	3.702548	0.714550
H	3.185728	2.052372	1.591224
H	4.059719	-0.274619	1.684871
H	4.126416	-2.584802	0.773049
H	2.612970	-3.213136	-1.150548
H	0.969418	-1.564274	-2.028325
N	-2.484447	1.279627	-0.332041
H	-3.438893	0.837128	-0.482372
H	-2.571089	2.294019	-0.260132
H	-2.024299	0.929704	0.550673
H	-1.783194	1.054601	-1.113633
N	-3.542525	-1.345752	1.712621
H	-3.154492	-0.649682	2.352347
H	-3.738504	-2.166578	2.288092
H	-2.755847	-1.607128	1.094765
N	-0.761992	0.357128	1.769390
H	-0.327070	-0.359294	1.175532
H	-0.040946	1.083302	1.840660
H	-0.824191	-0.069508	2.695933
N	-4.978707	-0.015833	-0.508089
H	-5.871503	0.444491	-0.325575
H	-5.149245	-0.661091	-1.281195
H	-4.754000	-0.594878	0.321337
N	-1.395411	-1.994152	-0.426487
H	-1.092833	-1.216773	-1.030650
H	-0.516721	-2.463746	-0.186074
H	-1.869631	-2.646904	-1.055276

(Vd)

La state optimized

Atom	X	Y	Z
C	0.999252	1.430465	-1.121280
C	0.918800	2.638810	-0.306331
C	1.248448	2.619563	1.036740
C	1.691177	1.422772	1.621976

C	1.825433	0.204866	0.874927
C	2.324778	-0.978678	1.500422
C	2.598057	-2.111394	0.674883
C	2.236817	-2.120632	-0.657304
C	1.572443	-1.008209	-1.256511
C	1.459325	0.193467	-0.484395
O	0.641030	1.465041	-2.318497
H	0.586368	3.543208	-0.817729
H	1.179880	3.526393	1.639666
H	1.968449	1.411454	2.678056
H	2.674197	-0.935287	2.532004
H	3.101317	-2.979991	1.104084
H	2.468874	-2.995056	-1.270038
H	1.417816	-0.950246	-2.332605
N	-1.660497	0.551586	0.444647
H	-2.594185	0.859530	0.832436
H	-0.926655	1.246500	0.618705
H	-1.364346	-0.380989	0.853885
H	-1.732316	0.369894	-0.587878
N	-3.749367	-1.585101	-0.117293
H	-2.982463	-1.984788	0.432177
H	-4.324295	-2.378563	-0.405674
H	-3.289668	-1.249154	-0.970274
N	-0.654285	-1.989583	1.111171
H	-0.199300	-2.154062	0.202304
H	0.159922	-1.753080	1.701403
H	-0.966057	-2.907572	1.435509
N	-4.308513	1.003629	1.323582
H	-4.599023	0.958545	2.301119
H	-4.934169	1.672907	0.873234
H	-4.498916	0.080051	0.905553
N	-1.559941	-0.401349	-2.283117
H	-0.904576	0.323630	-2.613176
H	-0.936907	-1.204453	-2.134381
H	-2.151143	-0.639648	-3.082094

(Ve)

Ground state optimized

Atom	X	Y	Z
C	0.315286	-1.550430	0.259528
C	0.826906	-1.273540	1.505833
C	0.040033	-0.609709	2.468736
C	-1.244270	-0.229269	2.196921
C	-1.799161	-0.492917	0.920619
C	-3.109497	-0.081802	0.575586
C	-3.609766	-0.304469	-0.676685
C	-2.825541	-0.959208	-1.650617
C	-1.559447	-1.377434	-1.346935
C	-1.017954	-1.152354	-0.061052
O	1.011786	-2.186597	-0.694097
H	1.837591	-1.575017	1.742810
H	0.467484	-0.411710	3.443428
H	-1.847097	0.274615	2.940685
H	-3.707187	0.421677	1.325135
H	-4.611371	0.019719	-0.925608
H	-3.231583	-1.130320	-2.638239
H	-0.948782	-1.884952	-2.079797
N	3.645594	-1.688658	-0.434649
H	3.669699	-1.111006	-1.271180
H	4.402516	-2.358566	-0.473361
H	3.811812	-1.035477	0.330099
H	1.997476	-2.135409	-0.504355
N	3.155657	0.980628	0.904662
H	3.648313	1.858022	1.019096
H	2.793151	0.962601	-0.048254
H	2.345510	1.012850	1.512845
N	1.968702	0.404348	-2.120278
H	1.281649	1.016855	-1.672275
H	2.101914	0.743278	-3.065307
H	1.520937	-0.504821	-2.186449
N	-0.097627	1.983773	-0.395748
H	-1.012629	1.708956	-0.737816

H	-0.011211	1.555867	0.520848
H	-0.106960	2.993326	-0.265823
N	0.052048	5.238578	-0.214335
H	0.928980	5.439707	-0.679132
H	0.082360	5.697149	0.687782
H	-0.677004	5.691528	-0.751540

(Ve)

Lb state optimized

Atom	X	Y	Z
C	0.965696	-0.767319	-1.176018
C	1.846914	-1.707082	-0.495371
C	1.354458	-2.576722	0.462441
C	-0.005868	-2.532147	0.814464
C	-0.924641	-1.634873	0.187397
C	-2.289565	-1.571647	0.570185
C	-3.186425	-0.727726	-0.137649
C	-2.732696	0.033683	-1.207046
C	-1.356531	0.033234	-1.563428
C	-0.448138	-0.789268	-0.854262
O	1.436898	0.069756	-2.004080
H	2.890950	-1.716783	-0.802532
H	2.001372	-3.317091	0.933719
H	-0.392808	-3.227022	1.569837
H	-2.664473	-2.217234	1.372582
H	-4.234711	-0.709636	0.158751
H	-3.422665	0.635737	-1.801584
H	-0.991405	0.589762	-2.430053
N	3.169048	1.491815	-0.608455
H	2.412349	2.242459	-0.563041
H	4.087914	1.848012	-0.862638
H	3.145926	1.028274	0.362876
H	2.770407	0.818231	-1.321140
N	2.645851	0.391694	1.866196
H	3.130486	0.550049	2.752442
H	1.675328	0.734603	1.994085

H	2.544937	-0.624140	1.770693
N	0.693557	2.647411	-0.461169
H	0.341599	2.243369	0.412842
H	0.155122	3.499093	-0.605955
H	0.388902	1.983069	-1.184665
N	-0.327317	1.050955	2.203330
H	-0.654261	0.178833	1.777561
H	-0.469584	0.917181	3.210717
H	-1.035799	1.744877	1.920285
N	-2.487879	2.668635	0.758402
H	-3.294700	2.149252	1.085289
H	-2.235141	2.188970	-0.118064
H	-2.836974	3.587721	0.488231

(Ve)

La state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	1.261452	-0.13844	-1.227457
C	2.549118	-0.644151	-0.778176
C	2.631241	-1.743278	0.055517
C	1.446183	-2.366965	0.48229
C	0.150642	-1.937664	0.052149
C	-1.033559	-2.573549	0.536224
C	-2.288165	-2.178228	-0.004273
C	-2.376277	-1.156623	-0.930765
C	-1.21515	-0.429135	-1.338886
C	0.052981	-0.863083	-0.853949
O	1.195069	0.940288	-1.878801
H	3.435736	-0.117534	-1.137274
H	3.59907	-2.128872	0.379764
H	1.504504	-3.226636	1.153366
H	-0.954911	-3.412093	1.227346
H	-3.192593	-2.710382	0.29872
H	-3.347459	-0.909147	-1.367536
H	-1.249033	0.291056	-2.154321
N	1.754334	2.81933	0.007297

H	0.699001	3.034763	-0.042625
H	2.319446	3.667206	0.015285
H	1.955123	2.185325	0.871191
H	1.918365	2.255753	-0.852642
N	2.032008	1.073026	2.091157
H	2.377342	1.305408	3.023777
H	1.030117	0.806463	2.195436
H	2.514239	0.216161	1.807282
N	-0.925886	2.937153	-0.529971
H	-1.732805	2.696294	0.0649
H	-1.260414	3.655852	-1.175923
H	-0.779216	2.096915	-1.106911
N	-0.851249	0.435709	1.961655
H	-1.006441	0.630702	0.965697
H	-1.056781	-0.568439	2.030921
H	-1.612249	0.919755	2.441376
N	-3.493377	1.593582	0.587308
H	-3.185114	0.614318	0.561021
H	-4.025949	1.708473	-0.278635
H	-4.192121	1.641447	1.332035

(Vf)

Ground state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.430165	-0.800118	1.030613
C	0.526474	-2.054128	0.471925
C	1.572776	-2.358587	-0.422465
C	2.515592	-1.427428	-0.757966
C	2.440424	-0.124103	-0.208497
C	3.367159	0.888785	-0.555944
C	3.250878	2.152700	-0.048879
C	2.201786	2.469476	0.840717
C	1.294821	1.512308	1.203473
C	1.390835	0.200006	0.687413
O	-0.531603	-0.453431	1.895564
H	-0.203975	-2.807274	0.731619

H	1.626831	-3.356443	-0.838839
H	3.320003	-1.667206	-1.440440
H	4.170275	0.642101	-1.239105
H	3.965393	2.915780	-0.327183
H	2.119942	3.472813	1.235858
H	0.488525	1.736687	1.886910
N	-2.758344	-1.917755	1.517010
H	-3.223150	-1.130989	1.067273
H	-3.354627	-2.288024	2.245300
H	-2.661487	-2.610583	0.777526
H	-1.299608	-1.102101	1.853973
N	-2.147005	-2.410561	-1.407197
H	-2.692980	-2.573147	-2.244677
H	-2.270396	-1.428877	-1.157328
H	-1.172738	-2.523115	-1.662085
N	-2.564823	0.653350	-0.257714
H	-1.917681	0.791394	-1.033235
H	-3.287290	1.366639	-0.322862
H	-2.022883	0.841252	0.580323
N	-0.084394	0.541199	-2.240213
H	0.568387	1.240608	-1.901943
H	0.262999	-0.347169	-1.890546
H	0.003201	0.516125	-3.248882
N	-4.851102	3.026073	-0.481744
H	-5.656053	2.950741	0.127654
H	-5.201839	3.070429	-1.430563
H	-4.413817	3.918203	-0.286593

(Vf)

Lb state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	-0.409782	-0.724944	-1.033444
C	-0.559675	-2.053786	-0.554080
C	-1.641031	-2.374530	0.303911
C	-2.563871	-1.392845	0.695975
C	-2.450521	-0.053207	0.252967

C	-3.338491	0.967237	0.651618
C	-3.192430	2.280549	0.206681
C	-2.121881	2.609975	-0.683392
C	-1.221651	1.631302	-1.097363
C	-1.338181	0.298139	-0.654722
O	0.584284	-0.386544	-1.826603
H	0.146254	-2.815433	-0.879884
H	-1.770494	-3.401684	0.646825
H	-3.396355	-1.660825	1.350680
H	-4.157555	0.708063	1.327150
H	-3.894590	3.049511	0.526508
H	-2.015382	3.632377	-1.046527
H	-0.409888	1.878719	-1.782673
N	2.639176	-1.853078	-1.475466
H	3.222894	-1.061872	-1.162176
H	3.148282	-2.390260	-2.176351
H	2.513403	-2.435399	-0.630208
H	1.381574	-1.098231	-1.787459
N	1.970541	-2.874739	1.278072
H	2.661162	-3.093017	1.999310
H	1.588509	-1.951680	1.529314
H	1.198747	-3.526020	1.437227
N	2.952379	0.688625	-0.078117
H	2.490962	0.299816	0.750084
H	3.393131	1.564952	0.225155
H	2.173727	0.957646	-0.687202
N	0.510198	-0.122954	2.027086
H	0.324108	0.603620	1.328460
H	-0.356156	-0.670444	2.034879
H	0.529060	0.366663	2.924348
N	4.254291	3.506127	0.771151
H	4.898945	3.776058	0.025742
H	4.806253	3.547104	1.629807
H	3.588127	4.277476	0.841838

(Vf)

La state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	1.101260	0.334124	-1.252695
C	2.537993	0.261997	-1.032248
C	3.096627	-0.787201	-0.328351
C	2.257851	-1.792937	0.183304
C	0.842063	-1.800862	-0.030557
C	0.022360	-2.842366	0.502269
C	-1.354392	-2.874007	0.143484
C	-1.914550	-1.875969	-0.629008
C	-1.137713	-0.755084	-1.064255
C	0.262086	-0.763327	-0.786230
O	0.590656	1.349222	-1.797964
H	3.141788	1.068443	-1.453095
H	4.174550	-0.843369	-0.170191
H	2.696031	-2.620724	0.745078
H	0.477859	-3.656076	1.065716
H	-1.973602	-3.710909	0.472682
H	-2.966070	-1.947014	-0.920411
H	-1.523097	-0.021515	-1.771016
N	0.826513	3.359921	-0.024978
H	-0.235457	3.240140	0.160760
H	1.149347	4.325258	-0.036015
H	1.273833	2.763684	0.750538
H	0.985343	2.862038	-0.926852
N	1.587916	1.524705	1.908128
H	1.960232	1.765744	2.829069
H	0.716059	0.993262	2.088512
H	2.236576	0.834948	1.517190
N	-1.591424	2.331437	0.472238
H	-1.535131	1.935237	1.415822
H	-2.593376	2.438627	0.277047
H	-1.321957	1.539358	-0.131871
N	-0.896183	-0.235000	2.296753
H	-1.348335	-0.336788	1.379259
H	-0.397358	-1.129820	2.375687

H	-1.656805	-0.299586	2.977387
N	-4.148038	0.959949	-0.452611
H	-4.128986	0.974122	-1.475382
H	-5.081202	0.619355	-0.212394
H	-3.508491	0.198509	-0.204799

(Vg)

Ground state optimized

Atom	X	Y	Z
C	1.029518	-0.133164	-1.376778
C	1.092656	-1.527840	-1.596955
C	-0.020012	-2.353631	-1.424462
C	-1.244142	-1.865149	-1.014749
C	-1.403371	-0.465391	-0.854961
C	-2.647698	0.116167	-0.497885
C	-2.801488	1.475118	-0.421678
C	-1.715513	2.331259	-0.700349
C	-0.491656	1.793491	-1.006892
C	-0.298654	0.399961	-1.071625
O	2.047403	0.624512	-1.401447
H	2.044233	-1.945072	-1.899973
H	0.089619	-3.417434	-1.601465
H	-2.099413	-2.518641	-0.900456
H	-3.491532	-0.539504	-0.315656
H	-3.766542	1.895658	-0.170000
H	-1.853517	3.403620	-0.673263
H	0.357636	2.424224	-1.231999
H	3.165568	-0.318042	-0.167631
N	3.454244	-0.863429	0.656759
H	4.156642	-0.326236	1.150608
H	3.913374	-1.699583	0.315252
H	1.819497	-1.147104	1.385735
N	0.791538	-1.241434	1.593860
H	0.567279	-1.881765	2.350767
H	0.355400	-0.300194	1.842862
H	0.325183	-1.594767	0.752928

N	-0.320271	1.241338	2.219548
H	0.479320	1.801535	1.901196
H	-1.103669	1.487468	1.621466
H	-0.549566	1.514737	3.166938
N	2.162309	2.454027	0.915147
H	3.096759	2.434072	1.305950
H	2.171205	1.875515	0.066613
H	2.004880	3.408457	0.611840
N	-1.862591	-1.955249	2.422230
H	-2.064141	-2.453095	1.561096
H	-2.587889	-2.200438	3.085132
H	-1.983998	-0.971194	2.198826

(Vg)

Lb state optimized

Atom	X	Y	Z
C	-0.743876	-0.042804	-1.467525
C	-0.867930	1.366942	-1.744266
C	0.240379	2.240525	-1.581531
C	1.424139	1.777660	-0.996528
C	1.581967	0.415994	-0.596057
C	2.763342	-0.074281	0.002713
C	2.966086	-1.431085	0.217167
C	1.972706	-2.372379	-0.232173
C	0.795961	-1.916703	-0.803142
C	0.529697	-0.543583	-0.949725
O	-1.736171	-0.814894	-1.60092
H	-1.817241	1.713228	-2.155181
H	0.166613	3.281081	-1.902411
H	2.270068	2.460392	-0.868223
H	3.547247	0.641185	0.271103
H	3.892523	-1.784165	0.669517
H	2.159076	-3.442840	-0.138866
H	0.046698	-2.623241	-1.166701
H	-3.222464	0.026637	-0.499197
N	-3.702173	0.480618	0.29312

H	-4.412038	-0.182987	0.609138
H	-4.224877	1.256589	-0.118464
H	-2.192827	0.966124	1.332121
N	-1.165301	1.127585	1.4413
H	-0.889161	1.984363	1.946515
H	-0.647332	0.260566	1.86309
H	-0.829010	1.259801	0.474119
N	0.115364	-1.097510	2.333097
H	-0.515262	-1.810251	1.925537
H	1.014302	-1.211231	1.853576
H	0.267960	-1.344975	3.311555
N	-1.911838	-2.711376	0.784804
H	-2.900115	-2.866687	0.992914
H	-1.890086	-2.123263	-0.060896
H	-1.561357	-3.620977	0.476537
N	0.722710	3.214377	1.933724
H	0.670738	3.685193	1.026217
H	1.137778	3.889107	2.578185
H	1.431983	2.487926	1.791264

(Vg)

La state optimized

<u>Atom</u>	<u>X</u>	<u>Y</u>	<u>Z</u>
C	0.436709	1.399560	-0.879133
C	1.170601	2.491834	-0.259088
C	2.362245	2.263284	0.398667
C	2.869307	0.956647	0.471476
C	2.197106	-0.164824	-0.117788
C	2.708352	-1.489587	0.037120
C	2.044345	-2.556042	-0.635852
C	0.890775	-2.334992	-1.357211
C	0.299840	-1.035125	-1.432716
C	1.004704	0.055060	-0.828388
O	-0.688143	1.613416	-1.398359
H	0.732020	3.487166	-0.345006
H	2.912606	3.087038	0.855117

H	3.814565	0.775027	0.988538
H	3.664586	-1.645539	0.537021
H	2.463424	-3.562997	-0.585964
H	0.418544	-3.167979	-1.882676
H	-0.489842	-0.811762	-2.149196
H	-1.997227	2.380331	-0.077519
N	-2.586165	2.110936	0.720466
H	-3.492467	1.867265	0.315015
H	-2.732840	2.946271	1.287782
H	-1.744019	0.525792	1.109157
N	-1.410739	-0.470356	1.168213
H	-0.633588	-0.589993	1.872646
H	-2.256293	-1.050561	1.362414
H	-1.022401	-0.744328	0.240609
N	-4.053695	-1.572977	1.109418
H	-4.052679	-1.057423	0.216493
H	-4.338452	-2.529237	0.892414
H	-4.808405	-1.181230	1.674681
N	-3.157557	-0.172785	-1.507939
H	-3.725356	0.191966	-2.276924
H	-2.316661	0.423861	-1.498645
H	-2.806085	-1.069296	-1.857121
N	0.931087	-0.786780	2.737950
H	1.413118	0.112818	2.810818
H	1.035513	-1.239609	3.647232
H	1.502650	-1.326067	2.070695