Table S1: B3LYP/6-31+G(d,p) Optimized Geometries in Cartesian Coordinates (Å) and Total Energies (a.u.) of All Radical Species

$R1^z$-I

E_{total}=-476.39955 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
N	.000108	1.337854	.460912
C	.590777	-.012195	.764574
C	-.543097	-1.010197	.485269
C	-1.516639	-.274158	-.447002
C	-1.429387	1.174324	.068350
C	1.855718	-.184042	-.135826
O	2.499900	-1.244231	.027618
O	-2.819638	-.829001	-.315948
O	2.090184	.787771	-.918531
H	.113566	1.982720	1.297431
H	.629645	1.668787	-.309639
H	-.160681	-1.939157	.057317
H	-1.090729	-1.249607	1.406601
H	-2.045638	1.280312	.968892
H	-1.712485	1.943535	-.654289
H	-1.181694	-.333002	-1.491179
H	-3.365986	-.592630	-1.077166
H	.905442	-.004638	1.818346

$R1^z$-II

E_{total}=-476.38726 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
N	.005364	1.385276	.445933
C	.597308	.049665	.830927
C	-.553172	-.946827	.667637
C	-1.427864	-.304846	-.420451
C	-1.380726	1.173798	-.050208
C	1.803105	-.210490	-.140444
O	2.342154	-1.329170	-.039001
O	-2.802392	-.724854	-.429374
O	2.070029	.762179	-.911647
H	.003202	2.073851	1.255958
H	.690273	1.694089	-.292049
H	-.162052	-1.933267	.405308
H	-1.145759	-1.019901	1.591177
H	-2.067526	1.386509	.784908
H	-1.601288	1.862284	-.868169
H	-.993804	-.473653	-1.416598
H	-2.829289	-1.643852	-.732860
H	.958464	.123976	1.866198

R1^A-I

E_{total}=-476.39047 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.317736	1.214722	-.139913
N	.034283	1.400991	.450555
C	.559094	.060366	.827427
C	-.616492	-.908645	.712305
C	-1.449934	-.296833	-.413319
C	1.726268	-.300800	-.087869
O	2.214867	.760945	-.764885
O	-2.799660	-.766992	-.352964
O	2.228200	-1.411321	-.159578
H	-.016784	1.986089	1.295889
H	-.296822	-1.934080	.513499
H	-1.202136	-.891607	1.645314
H	-2.100118	1.508746	.575649
H	-1.439366	1.813534	-1.051202
H	-1.030324	-.547816	-1.401660
H	-3.214559	-.603213	-1.221103
H	.954237	.111406	1.865480
H	1.551434	1.476093	-.548110

R1^A-II

E_{toatl}=-476.37979 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	1.878477	-.204449	.396396
C	1.562182	1.228022	-.093259
N	.127598	1.351604	.161092
C	-.447331	.086263	-.292774
C	.533408	-.957810	.275767
C	-1.908561	-.044301	.053853
O	-2.361652	-1.348960	-.074715
O	2.910953	-.840426	-.362170
O	-2.710999	.898492	.060275
H	-.309913	2.151341	-.288237
H	.186928	-1.305240	1.257824
H	.635846	-1.826921	-.377452
H	1.833098	1.289513	-1.161521
H	2.132580	1.993807	.453707
H	2.193974	-.167730	1.448032
H	3.757788	-.654023	.086613
H	-.409111	.010591	-1.412197
H	-3.329833	-1.271764	-.161430

R1^A-III

E_{total}=-476.37942 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	1.889890	-.191348	.387801
C	1.510932	1.251194	-.017684
N	.068330	1.297876	.226026
C	-.443212	.027717	-.306163
C	.584653	-.997367	.202237
C	-1.879839	-.270268	.037359
O	-2.394485	-1.394953	.025288
O	2.957615	-.729719	-.399596
O	-2.671409	.862805	-.037695
H	-.385633	2.099150	-.207216
H	.243649	-1.427792	1.151246
H	.737034	-1.814734	-.506146
H	1.787511	1.387190	-1.077036
H	2.038475	2.010532	.577874
H	2.196081	-.207655	1.442908
H	3.790394	-.524920	.064280
H	-.408602	.036051	-1.427799
H	-3.585533	.532416	-.125584

R1^A-IV

E_{total}=-476.37528 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	0.522731	-0.967266	0.256051
C	1.879395	-0.223648	0.379584
C	1.546548	1.249453	0.066540
N	0.096644	1.334179	0.256427
C	-0.446041	0.092709	-0.293859
O	2.886795	-0.693923	-0.513264
C	-1.936220	-0.040179	-0.031688
O	-2.709966	0.899919	-0.125209
O	-2.440628	-1.315597	0.049245
H	-0.330366	2.157646	-0.158367
H	0.196684	-1.319816	1.247040
H	0.620931	-1.839238	-0.395509
H	1.873427	1.454449	-0.966333
H	2.066856	1.949370	0.737766
H	2.256038	-0.322230	1.407309
H	3.441901	-1.326286	-0.015062
H	-0.366895	0.071649	-1.407626
H	-1.723170	-1.954409	0.209856

$R1^P$-I

E_{total}=-476.94340 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.456131	1.202428	-.066031
N	-.082109	1.358770	.469424
C	.496490	.010934	.733328
C	-.669160	-.979347	.585954
C	-1.579631	-.282518	-.438103
C	1.606194	-.218770	-.277510
O	2.319669	.898242	-.630569
O	-2.954894	-.654661	-.370962
O	2.403624	-1.294377	.025052
H	-.082087	1.920496	1.312733
H	1.660009	1.623194	-.568132
H	-.335623	-1.972385	.271215
H	-1.215864	-1.073683	1.531541
H	-2.221859	1.428164	.687449
H	-1.619487	1.858789	-.926046
H	-1.194537	-.448272	-1.453395
H	-3.060684	-1.539938	-.741671
H	.935396	-.021930	1.744403
H	3.175741	-1.275833	-.558063

$R1^P$-II

E_{total}=-476.94275 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.472403	1.204294	-.018519
N	-.079997	1.356850	.463488
C	.495911	.005078	.723193
C	-.667275	-.985339	.559545
C	-1.587697	-.276461	-.435803
C	1.613705	-.218414	-.280545
O	2.319939	.903072	-.637159
O	-2.912600	-.793328	-.334246
O	2.418741	-1.284429	.032774
H	-.041839	1.932547	1.296698
H	1.652357	1.621335	-.588981
H	-.339801	-1.968654	.214869
H	-1.209030	-1.108675	1.504536
H	-2.209444	1.390418	.774233
H	-1.674597	1.894310	-.845802
H	-1.205611	-.413639	-1.456346
H	-3.426125	-.512570	-1.102046
H	.926288	-.037486	1.737459
H	3.185697	-1.273004	-.557212

R1^P-III

E_{total}=-476.93499 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	1.960041	-.212440	.389641
C	1.607621	1.245397	.026978
N	.167923	1.330190	.280027
C	-.390710	.069778	-.214693
C	.594275	-.956701	.377033
C	-1.830082	-.111084	.192873
O	-2.429635	-1.331956	-.101897
O	2.887847	-.690385	-.589460
O	-2.622787	.921187	-.227927
H	-.270361	2.142466	-.143279
H	-3.547139	.688701	-.057698
H	.293741	-1.206320	1.401482
H	.657316	-1.876075	-.212864
H	1.882032	1.390152	-1.031673
H	2.153001	1.978023	.629209
H	2.418541	-.270726	1.384372
H	3.251543	-1.534992	-.294523
H	-.346882	.003442	-1.324744
H	-1.997516	-2.026469	.412807

R1^P-IV

E_{total}=-476.93487 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	1.938526	-0.199902	0.398946
C	1.591308	1.244110	-0.036073
N	0.160530	1.333423	0.247960
C	-0.407891	0.077444	-0.251058
C	0.600272	-0.968178	0.272243
C	-1.829821	-0.121522	0.205994
O	-2.436131	-1.333723	-0.106138
O	2.914222	-0.828167	-0.436890
O	-2.641373	0.920739	-0.150042
H	-0.288041	2.151190	-0.153772
H	-3.557781	0.677948	0.046583
H	0.285672	-1.343622	1.252015
H	0.725430	-1.814242	-0.408268
H	1.836892	1.339766	-1.109509
H	2.146607	2.008007	0.519097
H	2.287157	-0.211178	1.439059
H	3.769764	-0.399971	-0.302296
H	-0.408914	0.042625	-1.363272
H	-1.968602	-2.046993	0.348892

$R2^{C}$-I

E_{total}=-287.53083 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
N	1.178810	-.688011	-.359840
C	1.241629	.789569	-.293169
C	.011335	1.308378	.367997
C	-.893182	.053675	.479843
C	.113490	-1.080028	.663196
O	-1.527877	-.239310	-.757340
H	.862074	-.997136	-1.291957
H	.236189	1.724227	1.362698
H	-.462480	2.111382	-.208151
H	-.284047	-2.065055	.420071
H	.584072	-1.073734	1.647490
H	-1.601177	.104498	1.312703
H	-2.287665	.339414	-.910923
H	2.085309	-1.133952	-.181839
H	1.999437	1.291347	-.879690

$R2^{C}$-II

E_{total}=-287.53005 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
N	1.170818	-.707332	-.364879
C	1.259535	.768727	-.280752
C	.031121	1.300723	.372098
C	-.890103	.064881	.477363
C	.104447	-1.091972	.657546
O	-1.531828	-.084557	-.783231
H	.843908	-.997485	-1.299780
H	.254634	1.715611	1.366600
H	-.443149	2.096302	-.212358
H	-.295091	-2.076547	.413956
H	.580416	-1.097713	1.640520
H	-1.598291	.129277	1.307435
H	-2.405551	-.488066	-.689343
H	2.070033	-1.171511	-.197591
H	2.021986	1.263751	-.866964

$R2^{c}$-III

E_{total}=-287.52416 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	1.404074	.839529	-.049217
C	-.012727	1.268090	-.061624
C	-.805382	.010109	.387810
C	.069194	-1.164884	-.087211
N	1.498993	-.640945	.016951
H	2.092318	-1.024499	-.729459
H	-.182109	2.141760	.577967
H	-.344325	1.548063	-1.075830
H	-.138033	-1.366870	-1.140196
H	-.027880	-2.080641	.495454
O	-2.052991	-.145228	-.239336
H	-.899735	-.004913	1.481468
H	-2.759986	.261185	.279749
H	1.933608	-.941527	.899961
H	2.326155	1.398826	-.131632

$R2^{c}$-IV

E_{total}=-287.51971 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	1.392249	.848560	-.056229
C	-.031287	1.261356	-.066552
C	-.799813	-.011700	.375629
C	.087186	-1.168452	-.146330
N	1.505550	-.630485	.031597
H	2.150139	-1.012276	-.671706
H	-.220648	2.120494	.586202
H	-.347760	1.567660	-1.079412
H	-.065505	-1.334633	-1.215602
H	-.020653	-2.108923	.394093
O	-2.131104	-.118277	-.031832
H	-.832582	-.052309	1.469820
H	-2.237887	.093744	-.970979
H	1.887127	-.917139	.944113
H	2.307735	1.424401	-.062161

$R3^{Z}$

E_{total}=-475.74634 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.292125	1.135584	-.519168
N	-.193977	1.086872	.522198
C	.416350	-.310170	.507004
C	-.510750	-1.082988	-.354423
C	-1.782314	-.320637	-.574616
C	1.922871	-.140433	.011826
O	2.240196	1.065914	-.196738
O	-2.647812	-.601678	.533674
O	2.583857	-1.187818	-.071949
H	-.560238	1.335246	1.441825
H	.651638	1.666574	.272999
H	-.386751	-2.140121	-.543964
H	-2.056934	1.852106	-.216810
H	-.838727	1.447311	-1.462643
H	-2.272727	-.544395	-1.528214
H	-3.574558	-.439106	.299219
H	.462024	-.685201	1.538565

$R3^{N}$-I

E_{total}=-475.74732 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.222489	1.131448	-.509504
N	-.189082	1.137816	.557352
C	.393090	-.225882	.608781
C	-.532376	-1.094621	-.188064
C	-1.738368	-.311105	-.592904
C	1.838218	-.223364	.038345
O	2.292233	1.004615	-.242896
O	-2.812011	-.426174	.376974
O	2.482690	-1.234235	-.116730
H	-.617967	1.366441	1.448502
H	1.549719	1.613316	.001986
H	-.314928	-2.123444	-.447285
H	-2.017839	1.843770	-.279707
H	-.762891	1.415065	-1.463234
H	-2.117758	-.567242	-1.590038
H	-3.023627	-1.361994	.498596
H	.497118	-.563130	1.651011

$R3^N$-II

E_{total}=-475.74481 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.201942	1.131521	-.498352
N	-.172289	1.140408	.569809
C	.407551	-.225477	.619044
C	-.538876	-1.098823	-.144194
C	-1.735727	-.314513	-.568990
C	1.844514	-.226431	.026812
O	2.299239	1.001660	-.258726
O	-2.798693	-.548662	.384543
O	2.485217	-1.237428	-.138941
H	-.602625	1.364456	1.461668
H	-.393205	-2.159673	-.298390
H	-1.980724	1.867585	-.282437
H	-.732434	1.398287	-1.453664
H	-2.081657	-.581385	-1.576557
H	-3.634761	-.251390	-.001095
H	.527704	-.556209	1.661748
H	1.564499	1.613258	-.000874

$R3^N$-III

E_{total}=-475.74084 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.253087	1.188698	-.219870
N	-.335808	1.009461	.922982
C	.402946	-.231155	.658903
C	-.462781	-1.030725	-.290123
C	-1.668357	-.225767	-.661942
C	1.752964	.050916	-.018411
O	2.040829	1.026865	-.670279
O	-2.824786	-.596911	.134939
O	2.603474	-.994799	.161535
H	-.885719	.874000	1.766591
H	-.233357	-2.032856	-.636217
H	-2.115079	1.795994	.065199
H	-.715754	1.691049	-1.030524
H	-1.929216	-.285036	-1.726739
H	-2.994378	-1.541777	.019795
H	.620250	-.769474	1.590148
H	3.417678	-.791165	-.330029

$R3^N$-IV

E_{total}=-475.74087 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.215679	1.214603	.024917
N	-.258724	.800330	1.071054
C	.402244	-.424241	.581232
C	-.499921	-.967531	-.500839
C	-1.690213	-.076194	-.662145
C	1.810798	-.155516	.032126
O	1.864648	.928699	-.774546
O	-2.830056	-.565548	.093984
O	2.774563	-.856928	.255577
H	-.771280	.565132	1.915672
H	2.785633	1.017348	-1.073351
H	-.311396	-1.881181	-1.054893
H	-2.046839	1.772905	.461798
H	-.701814	1.853448	-.700605
H	-1.988684	.078392	-1.707202
H	-3.030524	-1.467801	-.190075
H	.559368	-1.137057	1.399426

$R3^N$-V

E_{total}=-475.73936 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.236414	1.187699	-.183480
N	-.313985	1.001854	.953248
C	.421515	-.238938	.670730
C	-.468175	-1.042794	-.248671
C	-1.660964	-.229759	-.636527
C	1.753875	.051169	-.036787
O	2.010930	1.018861	-.714492
O	-2.801302	-.731017	.101762
O	2.626268	-.974004	.147719
H	-.857862	.854391	1.799208
H	-.311756	-2.082381	-.510279
H	-2.086805	1.809434	.110124
H	-.697471	1.692367	-.992943
H	-1.877133	-.281863	-1.713329
H	-3.603242	-.334650	-.266817
H	.660217	-.777154	1.596390
H	3.425751	-.768101	-.366589

$R3^N$-VI

E_{total}=-475.73914 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.196766	1.205532	.090065
N	-.229335	.762223	1.113032
C	.422527	-.450762	.576472
C	-.509829	-.977406	-.484104
C	-1.686812	-.069417	-.634130
C	1.817969	-.149907	.010475
O	1.824337	.906069	-.836724
O	-2.815047	-.687539	.030356
O	2.812236	-.797630	.258023
H	-.730357	.499538	1.956790
H	-.400679	-1.934266	-.981015
H	-2.012646	1.765841	.555450
H	-.686220	1.862884	-.622667
H	-1.944937	.117691	-1.686249
H	-3.618162	-.208169	-.217081
H	.602319	-1.180293	1.374688
H	2.741286	1.025774	-1.137049

$R3^N$-VII

E_{total}=-475.73052 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.249657	1.193131	-.173380
N	-.324098	.978270	.956965
C	.418442	-.248144	.644586
C	-.451879	-1.020011	-.322559
C	-1.662621	-.206436	-.660691
C	1.768634	.069909	-.045285
O	1.995007	1.063532	-.682753
O	-2.810898	-.610916	.130297
O	2.707755	-.916069	.049692
H	-.867523	.813624	1.799737
H	-.213160	-1.995563	-.734065
H	-2.111901	1.786010	.139587
H	-.718621	1.724967	-.968521
H	-1.927404	-.230442	-1.725523
H	-3.008514	-1.539250	-.054009
H	.629976	-.805219	1.570188
H	2.413402	-1.625088	.639940

$R3^{N}$-VIII

E_{total}=-475.72941 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.230524	1.190071	-.166949
N	-.305492	.992081	.965753
C	.434565	-.239917	.663494
C	-.456595	-1.037003	-.259481
C	-1.652287	-.222496	-.636310
C	1.770638	.070381	-.056829
O	1.991742	1.066894	-.692147
O	-2.787740	-.738264	.098442
O	2.702607	-.923297	.011477
H	-.847133	.832842	1.811148
H	-.299012	-2.069078	-.551079
H	-2.081873	1.804973	.137495
H	-.693722	1.706468	-.969854
H	-1.868656	-.262924	-1.713232
H	-3.593537	-.346667	-.266815
H	.666148	-.777564	1.595522
H	2.408575	-1.641495	.590824

$R4^{Z}$-I

E_{total}=-475.74861 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.287882	1.193158	-.205997
N	.005810	1.269573	.553139
C	.549783	-.144060	.758982
C	-.596330	-1.105969	.384565
C	-1.761657	-.193390	.096872
C	1.838696	-.208097	-.143183
O	2.135934	.915519	-.666165
O	-2.873269	-.581309	-.580232
O	2.410101	-1.305431	-.226718
H	-.110190	1.774800	1.431222
H	.826386	1.653875	-.025532
H	-.318655	-1.700603	-.499735
H	-.804772	-1.816611	1.192753
H	-1.972530	1.980426	.120591
H	-1.066672	1.349830	-1.273429
H	-3.281157	-1.365302	-.184571
H	.849144	-.243505	1.804205

R4^{Z}-II

E_{total}=-475.75155 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
N	-.024054	1.264977	.466993
C	.542025	-.144377	.673753
C	-.540943	-1.091478	.128459
C	-1.783697	-.255919	.121697
C	-1.428157	1.195056	-.079248
C	1.906417	-.169303	-.098731
O	2.584434	-1.207413	.005848
O	-2.890744	-.803425	-.439017
O	2.136974	.897163	-.750665
H	.013209	1.816380	1.324123
H	.714719	1.626317	-.215083
H	-.283579	-1.434850	-.888206
H	-.645620	-1.985218	.749987
H	-2.070513	1.906643	.448484
H	-1.400886	1.483539	-1.141356
H	-3.685963	-.266996	-.293573
H	.707830	-.295128	1.741763

R4^{Z}-III

E_{total}=-475.74841 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.513351	-.279113	-.283190
C	-1.384140	1.199253	-.068419
N	.003200	1.335523	.499675
C	.570251	-.042411	.830522
C	-.590953	-1.027554	.635656
C	1.777824	-.210178	-.169796
O	2.360567	-1.303134	-.172144
O	-2.764873	-.696106	-.612021
O	2.006226	.846994	-.846840
H	.025595	1.979734	1.289193
H	.764108	1.596193	-.235666
H	-.212046	-1.966928	.218635
H	-1.082422	-1.262300	1.596640
H	-2.114678	1.580036	.660701
H	-1.471804	1.797137	-.980229
H	-2.858324	-1.654100	-.520102
H	.954024	-.040453	1.852503

$R4^{Z}$-IV

E_{total}=-475.75109 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-1.476543	1.174769	.066827
N	-.030896	1.322461	.455280
C	.573642	-.044985	.781000
C	-.546959	-1.062652	.501857
C	-1.557925	-.284379	-.285415
C	1.830033	-.166952	-.157711
O	1.987379	.836389	-.921812
O	-2.742696	-.899691	-.537018
O	2.509802	-1.201747	-.042031
H	.087283	1.999527	1.209256
H	.637951	1.574029	-.350919
H	-.154252	-1.929225	-.038617
H	-.993117	-1.437327	1.438083
H	-2.103496	1.444391	.932120
H	-1.710459	1.864588	-.750348
H	-3.414722	-.292796	-.881879
H	.897708	-.054827	1.822876

$R5^{A}$-I

E_{total}=-476.41925 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-.822149	-.688503	.923326
C	-1.902966	-.315676	-.045517
O	-2.043684	-1.043107	-1.069720
C	.498206	-1.207647	.455204
C	1.612865	-.142186	.313181
O	2.806893	-.767210	-.215842
C	1.233257	1.069905	-.556888
N	.430623	2.060881	.174707
O	-2.540219	.745056	.255015
H	-.929661	-.364342	1.957887
H	.890116	-1.986706	1.128076
H	.332498	-1.666041	-.531637
H	1.905411	.234097	1.299631
H	2.533017	-1.308364	-.969208
H	.748337	.703964	-1.479880
H	2.177559	1.546916	-.846200
H	.359368	2.908948	-.381915
H	-.530202	1.732089	.308826

$R5^{A}$-II

E_{total}=-476.41656 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	-.822654	-.771396	.869324
C	.482068	-1.269071	.331430
C	1.583323	-.190599	.292922
C	1.232945	1.043774	-.560469
C	-1.919993	-.287580	-.029022
O	-2.448576	.814366	.336263
O	-2.182652	-.967384	-1.058882
N	.462886	2.043381	.193302
O	2.765026	-.844368	-.231516
H	-.890705	-.518477	1.927584
H	.876614	-2.100244	.936391
H	.326029	-1.642450	-.687497
H	1.788826	.161392	1.315502
H	3.466946	-.182652	-.285979
H	.742082	.701595	-1.486570
H	2.181950	1.518459	-.856145
H	.355337	2.877932	-.378525
H	-.491808	1.709091	.370090

$R5^{N}$-I

E_{total}=-476.97430 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	.796922	-.926056	-.455214
C	-.490285	-1.123750	.257754
C	-1.693621	-.327288	-.327476
C	-1.669882	1.167379	.036466
N	-.449655	1.826861	-.423656
C	1.908549	-.218754	.134196
O	3.041947	-.279547	-.621588
O	1.878365	.399753	1.198435
O	-2.926519	-.912986	.088378
H	.926014	-1.316770	-1.459734
H	-.777065	-2.181334	.178428
H	-.371962	-.880129	1.320570
H	-1.687480	-.424506	-1.417819
H	-3.020752	-.804126	1.045468
H	-1.822318	1.259110	1.126606
H	-2.536476	1.630419	-.445968
H	-.620225	2.783431	-.711761
H	.278177	1.825298	.284854
H	3.719230	.233644	-.151202

R5^{N}-II

E_{total}=-476.97384 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	.805674	-.944527	-.405600
C	-.476375	-1.090185	.331552
C	-1.671949	-.345921	-.308273
C	-1.706496	1.151608	.042545
N	-.510090	1.845053	-.435276
C	1.926146	-.202384	.123658
O	3.051991	-.321493	-.636566
O	1.907534	.489556	1.141120
O	-2.843462	-1.001263	.190054
H	.925364	-1.402739	-1.382626
H	-.759966	-2.151885	.335302
H	-.360750	-.770747	1.372004
H	-1.615061	-.449687	-1.402192
H	-3.626495	-.581066	-.189825
H	-1.868557	1.240419	1.128095
H	-2.582368	1.593263	-.450559
H	-.702898	2.812930	-.667500
H	.235693	1.825871	.255250
H	3.735156	.222334	-.211179

R5^{N}-III

E_{total}=-476.97134 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	0.799230	-0.888011	-0.543492
C	2.000001	-0.267292	-0.044728
O	1.863267	0.301183	1.203329
C	-0.456764	-1.112074	0.221821
C	-1.690677	-0.331255	-0.314087
O	-2.901447	-0.932168	0.143403
C	-1.671454	1.163007	0.051356
N	-0.469361	1.832543	-0.440944
O	3.070114	-0.220935	-0.641798
H	0.867556	-1.234661	-1.569525
H	-0.729078	-2.173975	0.139269
H	-0.311232	-0.886955	1.284642
H	-1.722193	-0.425837	-1.404260
H	-2.959761	-0.834662	1.104513
H	-1.794532	1.253429	1.145159
H	-2.555262	1.619676	-0.405055
H	-0.656458	2.773014	-0.767994
H	0.267118	1.870457	0.255589
H	2.741875	0.640823	1.439580

$R5^N$-IV

E_{total}=-476.97067 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	0.842512	-0.166116	-0.695867
C	-0.280903	-0.951440	-0.117767
C	-1.677884	-0.362236	-0.368945
C	-1.992264	0.884876	0.474974
N	-1.172879	2.032737	0.077923
C	2.161526	-0.057472	-0.116927
O	3.098167	0.548676	-0.630186
O	2.299084	-0.692644	1.088739
O	-2.590635	-1.418048	-0.046501
H	0.725794	0.333049	-1.651957
H	-0.286270	-1.951586	-0.585413
H	-0.131715	-1.126634	0.952920
H	-1.767455	-0.090193	-1.431405
H	-3.492898	-1.123723	-0.227932
H	-1.910067	0.613520	1.539776
H	-3.041790	1.150495	0.294785
H	-1.616517	2.910537	0.327563
H	-0.258555	2.019507	0.519405
H	3.218781	-0.553674	1.367575

$R5^N$-V

E_{total}=-476.96586 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	0.800085	-0.893349	-0.490112
C	-0.494255	-1.154058	0.189298
C	-1.689295	-0.308513	-0.338668
C	-1.616526	1.173659	0.069249
N	-0.399355	1.819439	-0.421442
C	1.897907	-0.216369	0.174948
O	3.084385	-0.131385	-0.500965
O	1.815401	0.292341	1.285388
O	-2.925348	-0.878277	0.086967
H	0.911138	-1.191832	-1.530823
H	-0.781344	-2.201701	0.025015
H	-0.381856	-0.993916	1.268198
H	-1.711517	-0.369053	-1.431884
H	-2.990192	-0.808952	1.050194
H	-1.715876	1.238680	1.165886
H	-2.493836	1.667691	-0.360480
H	-0.572851	2.760566	-0.754711
H	0.328945	1.853616	0.285225
H	3.019876	-0.560821	-1.365939

$R5^N$-VI

E_{total}=-476.96516 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	.811430	-.910967	-.428078
C	1.924041	-.187262	.161689
O	1.855621	.429678	1.216148
C	-.474755	-1.111864	.288991
C	-1.669298	-.339457	-.315762
O	-2.840067	-.985068	.194172
C	-1.670406	1.154059	.054511
N	-.474416	1.832585	-.447148
O	3.106589	-.187137	-.526186
H	.908065	-1.296626	-1.441588
H	-.750641	-2.174368	.233907
H	-.364901	-.847444	1.345122
H	-1.634348	-.427236	-1.412570
H	-3.624534	-.542957	-.156780
H	-1.797537	1.234303	1.144499
H	-2.553528	1.614637	-.407419
H	-.667425	2.788440	-.723992
H	.268950	1.845209	.245735
H	3.033592	-.708895	-1.338043

$R5^N$-VII

E_{total}=-476.96005 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	0.857223	-0.021509	-0.616359
C	-0.243773	-0.918715	-0.161190
C	-1.663841	-0.373047	-0.381179
C	-2.033330	0.818018	0.520271
N	-1.320395	2.038785	0.138425
C	2.212056	0.004805	-0.091255
O	3.048383	0.810194	-0.472705
O	2.560290	-0.899186	0.878114
O	-2.522040	-1.486134	-0.108751
H	0.684414	0.662821	-1.440057
H	-0.194740	-1.872408	-0.715390
H	-0.147200	-1.187279	0.901914
H	-1.763528	-0.055349	-1.429412
H	-3.436942	-1.236480	-0.293761
H	-1.895966	0.516821	1.571968
H	-3.105465	1.008023	0.385254
H	-1.811435	2.868229	0.455617
H	-0.382646	2.075138	0.526835
H	1.833198	-1.507330	1.073066

$R5^N$-VIII

E_{total}=-476.95862 a.u.

	Coordinates (Å)		
Atom	**X**	**Y**	**Z**
C	.849175	-.121406	-.679630
C	-.285397	-.961938	-.197597
C	-1.689070	-.339236	-.386417
C	-1.968882	.886882	.498817
N	-1.124901	2.029590	.153178
C	2.177844	-.040621	-.098162
O	3.017499	.758841	-.484144
O	2.497229	-.881751	.938117
O	-2.689596	-1.336561	-.174593
H	.710190	.497277	-1.559378
H	-.304076	-1.912494	-.757420
H	-.167600	-1.235475	.863503
H	-1.800974	-.038413	-1.432913
H	-2.734523	-1.549311	.768405
H	-1.892192	.582741	1.559987
H	-3.013257	1.163189	.324615
H	-1.581796	2.910661	.361560
H	-.230930	2.023778	.633252
H	1.786393	-1.515402	1.109033