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24				
I Energy= -680.584790529 Hartrees				
N	1.247565	-1.106689	0.000075	
C	1.853775	0.163739	0.000026	
N	1.013563	1.270389	0.000100	
C	-0.349039	1.091399	0.000058	
C	-0.907080	-0.171084	0.000086	
C	-0.142374	-1.379883	0.000009	
N	-2.277591	0.037107	-0.000090	
C	-2.445750	1.381119	0.000012	
N	-1.301758	2.058401	-0.000058	
C	2.180881	-2.240572	0.000007	
O	3.066355	0.286225	-0.000027	
C	1.624833	2.601105	-0.000058	
O	-0.592781	-2.518368	-0.000133	
C	-3.311394	-0.992318	0.000053	
H	-3.426840	1.831795	-0.000023	
H	1.592575	-3.153489	-0.000096	
H	2.816830	-2.196004	0.884308	
H	2.816907	-2.195838	-0.884227	
H	0.824527	3.336899	0.000151	
H	2.249907	2.722160	-0.885334	
H	2.250361	2.722134	0.884896	
H	-4.285276	-0.503359	-0.001073	
H	-3.212240	-1.620563	0.884800	
H	-3.210908	-1.622070	-0.883455	
24				
II Energy= -680.584339663 Hartrees				
N	1.250785	1.105003	-0.000778	
C	1.864608	-0.165026	0.000171	
N	1.018843	-1.268508	-0.000373	
C	-0.344690	-1.093116	-0.000512	
C	-0.906596	0.166995	-0.000374	
C	-0.137142	1.371880	-0.000166	
N	-2.276072	-0.044058	-0.000342	
C	-2.440864	-1.388853	-0.000452	
N	-1.295049	-2.062891	-0.000612	
C	2.124579	2.286236	-0.000243	
O	3.075339	-0.305385	0.001221	
C	1.628363	-2.600552	0.000244	
O	-0.569443	2.517410	0.000651	
C	-3.311153	0.983924	0.000705	
H	-3.420780	-1.842050	-0.000513	
H	1.929626	2.884841	0.890141	
H	1.911754	2.897376	-0.877717	
H	3.155327	1.947477	-0.012400	
H	0.826817	-3.334941	-0.000318	
H	2.252834	-2.722287	0.885764	
H	2.254201	-2.722420	-0.884285	
H	-4.284582	0.494121	-0.003505	
H	-3.209929	1.616023	-0.881107	
H	-3.214608	1.609902	0.887458	
24				
III Energy= -680.584509225 Hartrees				
N	1.263651	-1.092094	-0.000146	
C	1.861058	0.184258	-0.000115	
N	1.003373	1.281546	-0.000466	
C	-0.354989	1.080203	-0.000191	
C	-0.902617	-0.185650	-0.000168	
C	-0.122882	-1.384306	0.000100	
N	-2.273904	0.011964	0.000193	
C	-2.452494	1.355346	0.000251	
N	-1.313382	2.041564	0.000087	
C	2.208725	-2.216865	0.000007	
O	3.073726	0.302745	0.000110	
C	1.542863	2.642658	0.000064	
O	-0.558131	-2.528443	0.000328	
C	-3.299547	-1.025627	-0.000196	
H	-3.437318	1.797819	0.000461	

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H	1.629591	-3.135554	0.000142	
H	2.844212	-2.165686	0.884186	
H	2.844184	-2.165932	-0.884210	
H	1.201657	3.174512	0.889547	
H	1.194184	3.177694	-0.884534	
H	2.626668	2.573815	-0.004436	
H	-4.277345	-0.544615	0.003059	
H	-3.192775	-1.655834	0.882259	
H	-3.196687	-1.651590	-0.886178	
24				
IV Energy=		-680.583959073	Hartrees	
N	-1.268056	-1.089346	-0.000854	
C	-1.872708	0.187287	-0.000024	
N	-1.007899	1.280589	-0.000019	
C	0.351230	1.081408	-0.000365	
C	0.902040	-0.182454	-0.000537	
C	0.116836	-1.376989	0.000096	
N	2.272514	0.017341	0.000013	
C	2.448597	1.361587	0.000260	
N	1.307951	2.045017	0.000080	
C	-2.154112	-2.262249	-0.000531	
O	-3.083119	0.324514	0.000544	
C	-1.542727	2.644203	0.000210	
O	0.532085	-2.528246	0.001265	
C	3.298932	-1.019255	-0.000402	
H	3.432662	1.805949	0.000475	
H	-1.965151	-2.862694	0.890008	
H	-1.946738	-2.875573	-0.877889	
H	-3.181617	-1.914250	-0.013109	
H	-1.200126	3.174572	-0.889701	
H	-1.190301	3.177609	0.884374	
H	-2.626703	2.580214	0.006088	
H	4.276577	-0.537766	0.002339	
H	3.196413	-1.645476	-0.886436	
H	3.193149	-1.649157	0.882594	
24				
V Energy=		-680.584106516	Hartrees	
N	-1.254699	-1.101433	-0.000223	
C	-1.855659	0.171807	-0.000283	
N	-1.008652	1.272106	-0.000179	
C	0.352987	1.084759	-0.000134	
C	0.908792	-0.179418	-0.000224	
C	0.132946	-1.383582	-0.000225	
N	2.281486	0.028982	0.000046	
C	2.449948	1.372844	0.000052	
N	1.306844	2.050625	0.000098	
C	-2.194710	-2.230160	0.000088	
O	-3.067450	0.300058	0.000342	
C	-1.611563	2.606745	0.000178	
O	0.568889	-2.528566	0.000138	
C	3.330707	-0.991721	-0.000019	
H	3.430954	1.824355	0.000164	
H	-1.612543	-3.146938	-0.000318	
H	-2.830837	-2.181265	-0.883922	
H	-2.829994	-2.181573	0.884731	
H	-0.806966	3.337830	-0.000022	
H	-2.235832	2.731362	0.885620	
H	-2.236437	2.731504	-0.884812	
H	2.853075	-1.968575	0.000306	
H	3.950996	-0.888926	0.891943	
H	3.950538	-0.889302	-0.892344	
24				
VI Energy=		-680.583720599	Hartrees	
N	-1.256739	1.100577	0.000203	
C	-1.866267	-0.172316	0.000224	
N	-1.014849	-1.269994	0.000162	
C	0.348157	-1.087413	0.000097	
C	0.908044	0.174018	0.000149	
C	0.128931	1.375091	0.000093	

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N	2.279470	-0.037132	-0.000076	
C	2.444497	-1.381807	-0.000105	
N	1.299342	-2.056260	-0.000110	
C	-2.136760	2.277446	-0.000002	
O	-3.076203	-0.317097	-0.000193	
C	-1.617260	-2.605376	-0.000112	
O	0.549156	2.526042	-0.000140	
C	3.328557	0.983460	0.000020	
H	3.424168	-1.836136	-0.000210	
H	-3.165757	1.932865	0.000427	
H	-1.936410	2.883139	-0.884319	
H	-1.935852	2.883787	0.883736	
H	-0.812166	-3.335903	-0.000094	
H	-2.241711	-2.730325	-0.885324	
H	-2.241957	-2.730539	0.884892	
H	2.850331	1.960196	-0.000267	
H	3.949104	0.881046	-0.891829	
H	3.948665	0.881355	0.892212	
24				
VII Energy= -680.583854050 Hartrees				
N	1.270508	-1.086887	-0.000151	
C	1.862791	0.192105	-0.000619	
N	0.998585	1.283061	-0.000236	
C	-0.358713	1.073766	-0.000155	
C	-0.904245	-0.193653	-0.000095	
C	-0.113740	-1.387678	-0.000170	
N	-2.277570	0.004114	-0.000000	
C	-2.456525	1.347344	-0.000132	
N	-1.318224	2.034098	-0.000017	
C	2.222106	-2.206594	0.000295	
O	3.074631	0.316435	0.000354	
C	1.529681	2.647484	0.000010	
O	-0.534793	-2.538004	0.000111	
C	-3.318191	-1.025322	0.000313	
H	-3.441267	1.790644	-0.000095	
H	1.649026	-3.129044	0.000532	
H	2.857153	-2.151260	0.884653	
H	2.857302	-2.151782	-0.883987	
H	2.614041	2.585038	-0.000172	
H	1.181738	3.178736	0.887276	
H	1.181474	3.179119	-0.886920	
H	-2.832208	-1.998151	-0.000108	
H	-3.939430	-0.927890	-0.891517	
H	-3.938592	-0.928258	0.892769	
24				
VIII Energy= -680.583366377 Hartrees				
N	-1.273873	-1.084716	0.000008	
C	-1.873782	0.194193	0.000358	
N	-1.003927	1.281850	0.000128	
C	0.354504	1.075959	0.000059	
C	0.903390	-0.189142	-0.000023	
C	0.108418	-1.379074	0.000034	
N	2.275619	0.010542	-0.000006	
C	2.452041	1.354499	0.000099	
N	1.312072	2.038599	0.000045	
C	-2.165442	-2.253709	-0.000241	
O	-3.083727	0.335991	-0.000047	
C	-1.531474	2.648317	0.000111	
O	0.511870	-2.535780	-0.000043	
C	3.315403	-1.019499	-0.000254	
H	3.435765	1.799999	0.000109	
H	-3.191206	-1.900397	-0.000647	
H	-1.970520	-2.861434	0.883887	
H	-1.969814	-2.861555	-0.884123	
H	-2.615796	2.589932	0.000288	
H	-1.181255	3.178358	-0.886961	
H	-1.180975	3.178467	0.887007	
H	2.828223	-1.991911	0.000129	
H	3.936792	-0.922984	0.891593	

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H	3.936067	-0.923335	-0.892647	