Tuning the aromatic backbone twist in dipyrrolonaphthyridinediones

Cartesian coordinates

1								
S_0				S_1				
47				47				
FINAL HEAT OF FORMATION = -1070.269050				FINAL HEAT OF FORMATION = -1070.175120				
C	3.498328	1.705240	0.366828	C	3.557499	1.677039	0.262372	
C	2.226321	1.105268	0.242525	C	2.241143	1.104910	0.210720	
N	2.442280	-0.258772	0.070368	N	2.416538	-0.279968	0.072497	
C	3.795399	-0.534319	0.076146	C	3.752405	-0.586040	0.033050	
C	4.468435	0.673254	0.262849	C	4.474187	0.621216	0.149156	
C	0.899489	1.639293	0.224267	C	0.955982	1.653011	0.255064	
C	-0.174620	0.756183	0.053715	C	-0.171194	0.735338	0.140865	
C	0.046144	-0.690571	-0.019769	C	0.020024	-0.684918	0.067161	
C	1.422081	-1.231395	-0.110241	C	1.369170	-1.241890	-0.018965	
C	-1.030585	-1.585379	0.031903	C	-1.110200	-1.608325	0.070265	
C	-2.358208	-1.054942	0.075334	C	-2.394611	-1.058015	0.067507	
N	-2.571896	0.319820	0.043064	N	-2.568977	0.334093	0.072477	
C	-1.549054	1.304992	-0.010580	C	-1.521281	1.298908	0.095089	
C	-3.631874	-1.663409	0.105342	C	-3.711151	-1.631085	0.042486	
C	-4.600728	-0.625142	0.087976	C	-4.627143	-0.568344	0.028752	
C	-3.925189	0.594670	0.045854	C	-3.904724	0.643617	0.048286	
O	-1.870975	2.485098	-0.102884	O	-1.837501	2.495270	0.063734	
C	-0.916239	-3.088415	-0.001966	C	-0.994242	-3.107575	0.013529	
C	-0.865332	-3.615077	-1.447994	C	-0.849002	-3.615168	-1.435016	
C	-0.702367	-5.135518	-1.504998	C	-0.657555	-5.132048	-1.500193	
C	-0.669347	-5.664254	-2.940607	C	-0.537279	-5.642979	-2.937696	
O	1.747268	-2.395732	-0.319176	O	1.688201	-2.428965	-0.169645	
C	0.784803	3.137810	0.347267	C	0.841791	3.150520	0.357214	
C	0.771306	3.819278	-1.033863	C	0.724300	3.816431	-1.028614	
C	0.621010	5.336430	-0.912526	C	0.559574	5.332733	-0.913354	
H	4.141721	-1.558255	-0.048573	H	4.069617	-1.622918	-0.068463	
H	-4.269967	1.626410	0.021631	H	-4.221445	1.685611	0.051614	
H	5.551399	0.788561	0.317235	H	5.562720	0.697429	0.149737	
H	3.688227	2.769622	0.504299	H	3.780902	2.739646	0.359727	
H	-5.684515	-0.744344	0.104233	H	-5.715540	-0.643331	0.007543	
H	-3.823289	-2.736192	0.125073	H	-3.935118	-2.697924	0.025739	
H	-0.130109	3.412882	0.890907	H	-0.031363	3.432542	0.962473	
H	1.648273	3.508839	0.925896	H	1.745004	3.535669	0.863705	
H	-0.014871	-3.420203	0.532220	H	-0.130619	-3.451774	0.599710	
H	-1.793556	-3.518357	0.510878	H	-1.905162	-3.546162	0.458417	
H	-0.065334	3.406814	-1.622206	H	-0.144109	3.385978	-1.554727	
H	1.707059	3.567079	-1.566334	H	1.626889	3.569609	-1.618752	
H	-0.019004	-3.136837	-1.971294	H	0.019024	-3.117809	-1.901775	
H	-1.792013	-3.315552	-1.974446	H	-1.749118	-3.321758	-2.009843	
H	0.231742	-5.411992	-0.981689	H	0.251884	-5.397841	-0.929988	
H	-1.529928	-5.615092	-0.948134	H	-1.505496	-5.632326	-0.994415	
H	0.627621	5.819724	-1.903475	H	0.496118	5.805736	-1.907450	
H	-0.330237	5.591114	-0.415127	H	-0.362433	5.577935	-0.359246	

H	-0.543753	-6.759365	-2.966443	H	-0.390906	-6.735482	-2.968925
H	-1.604290	-5.417628	-3.472731	H	-1.446120	-5.406131	-3.517420
H	0.166131	-5.213782	-3.503348	H	0.319406	-5.171347	-3.448903
H	1.442946	5.771297	-0.317356	H	1.410614	5.786035	-0.375450

4							
S_0				S_1			
45				45			
FINAL HEAT OF FORMATION = -1069.040300				FINAL HEAT OF FORMATION = -1068.970630			
C	-3.914304	0.832006	1.098086	C	-3.894254	0.663299	1.404421
N	-2.610580	0.430428	0.876517	N	-2.622892	0.231102	1.075593
C	-2.587773	-0.840394	0.302076	C	-2.698239	-1.052483	0.508834
C	-3.930358	-1.250117	0.167567	C	-4.065289	-1.426174	0.503328
C	-4.747953	-0.205817	0.680758	C	-4.793658	-0.364039	1.100872
C	-1.469125	1.272484	0.943184	C	-1.529432	1.113658	0.766207
C	-0.205407	0.584631	0.596794	C	-0.274693	0.432457	0.268887
C	-0.158217	-0.864232	0.442479	C	-0.185634	-0.924317	0.573203
C	-1.341927	-1.486376	0.026686	C	-1.491471	-1.568455	0.017300
C	1.132311	-1.574723	0.316716	C	1.025126	-1.639777	0.617583
N	2.256815	-0.705937	0.263464	N	2.159472	-0.745822	0.474150
C	2.159800	0.670205	0.055715	C	2.085633	0.577360	-0.003921
C	0.886452	1.321290	0.125285	C	0.853491	1.217179	-0.146940
C	3.575576	-1.109373	0.175849	C	3.463911	-1.147630	0.532773
C	4.346645	0.028354	-0.064420	C	4.276961	-0.062688	0.125545
C	3.469103	1.144402	-0.156494	C	3.446422	1.005370	-0.222017
C	0.705258	2.610895	-0.640264	C	0.688630	2.529999	-0.871847
O	1.288408	-2.788867	0.298603	O	1.224900	-2.869885	0.681760
C	-1.316586	-2.463892	-1.130363	C	-1.343569	-2.257373	-1.297968
O	-1.577933	2.441073	1.292043	O	-1.608483	2.301520	1.023970
H	3.830506	-2.162515	0.278297	H	3.699820	-2.168697	0.829333
H	-4.117719	1.821139	1.504203	H	-4.047471	1.674814	1.780916
H	5.432846	0.043782	-0.160834	H	5.367926	-0.078828	0.095780
H	3.743185	2.188867	-0.309331	H	3.742699	2.008617	-0.529610
H	-5.836745	-0.202318	0.743072	H	-5.867546	-0.335074	1.291145
H	-4.261590	-2.217376	-0.211230	H	-4.450108	-2.393902	0.174936
C	1.157271	2.430177	-2.127758	C	1.276515	2.487775	-2.308797
H	-0.347520	2.919442	-0.583315	H	-0.383670	2.770493	-0.918043
H	1.295680	3.436684	-0.201300	H	1.165214	3.364413	-0.322946
C	-0.720831	-1.657899	-2.332374	C	-0.552637	-1.375419	-2.310563
H	-0.693254	-3.346511	-0.931940	H	-0.749486	-3.181304	-1.142228
H	-2.340845	-2.800096	-1.359570	H	-2.337199	-2.519606	-1.706847
C	0.970134	1.075344	-2.862992	C	1.081611	1.212459	-3.152891
H	0.671531	3.229543	-2.719854	H	0.864180	3.354176	-2.861217
H	2.240201	2.641029	-2.169011	H	2.366347	2.658873	-2.247897
C	-1.282209	-0.230154	-2.518782	C	-1.202824	-0.031221	-2.662186
H	0.371141	-1.600857	-2.167064	H	0.459567	-1.212731	-1.900065
H	-0.861783	-2.235525	-3.266311	H	-0.420871	-1.970013	-3.234669
H	-2.305817	-0.294301	-2.934339	H	-2.179460	-0.219697	-3.148904
H	-1.383450	0.273272	-1.545870	H	-1.428489	0.537213	-1.743393
C	-0.420975	0.677567	-3.418024	C	-0.344846	0.831309	-3.610318
H	1.656208	1.135173	-3.728015	H	1.678913	1.374431	-4.069660

H 1.377386 0.258568 -2.241066	H 1.565596 0.360607 -2.642930
H -0.269271 0.162766 -4.386031	H -0.247941 0.270624 -4.559914
H -0.995336 1.594337 -3.651525	H -0.903825 1.753563 -3.861450

5	
S_0	S_1
48	48
FINAL HEAT OF FORMATION = -1108.249140	FINAL HEAT OF FORMATION = -1108.161590
C -3.854087 0.714456 0.368681	C -3.831603 0.695600 0.453331
N -2.521272 0.361234 0.454339	N -2.510764 0.334039 0.485830
C -2.357574 -0.992977 0.164098	C -2.375695 -1.039672 0.204692
C -3.646108 -1.502041 -0.114112	C -3.706055 -1.533912 -0.023387
C -4.569634 -0.431082 0.021434	C -4.587235 -0.455339 0.140474
C -1.456450 1.276121 0.675883	C -1.427718 1.252597 0.631175
C -0.116732 0.655147 0.596064	C -0.111261 0.639413 0.506284
C 0.021734 -0.797667 0.610455	C 0.023049 -0.781324 0.519168
C -1.065891 -1.602107 0.255902	C -1.113745 -1.638259 0.224413
C 1.349031 -1.417107 0.814284	C 1.323362 -1.392330 0.763425
N 2.429607 -0.504154 0.676962	N 2.415331 -0.474721 0.702581
C 2.292668 0.846646 0.358336	C 2.305633 0.896041 0.397097
C 0.998182 1.456076 0.329384	C 1.046834 1.494203 0.302761
C 3.764610 -0.857677 0.712697	C 3.733868 -0.836146 0.786820
C 4.508413 0.283870 0.415278	C 4.514153 0.311827 0.527974
C 3.600937 1.353128 0.188577	C 3.650855 1.388546 0.279038
C 0.908644 2.875484 -0.186654	C 0.930164 2.895498 -0.233514
C 0.252618 2.927990 -1.595082	C 0.259822 2.924138 -1.639296
C 0.708770 1.804325 -2.559411	C 0.726959 1.796929 -2.591541
O 1.580567 -2.593482 1.064451	O 1.559339 -2.584354 0.994105
C -0.931892 -3.027071 -0.234484	C -0.953146 -3.045014 -0.285553
C -0.154844 -3.093709 -1.579304	C -0.161246 -3.093790 -1.626065
C -0.526081 -1.981373 -2.591955	C -0.534231 -1.977430 -2.631136
C 0.443920 -0.770245 -2.593464	C 0.442722 -0.773583 -2.623926
C -0.258163 0.592805 -2.630438	C -0.247322 0.593173 -2.665132
O -1.708336 2.455110 0.891782	O -1.682055 2.446741 0.828586
H 4.048224 -1.885402 0.931343	H 4.000681 -1.870624 0.999905
H -4.155181 1.744660 0.548897	H -4.115336 1.732060 0.632187
H 5.596729 0.332255 0.367190	H 5.605108 0.334439 0.521706
H 3.858728 2.384924 -0.048757	H 3.929087 2.423403 0.078696
H -5.649806 -0.481048 -0.119341	H -5.673711 -0.478754 0.041743
H -3.882461 -2.536419 -0.362295	H -3.966409 -2.570730 -0.237184
H 0.343026 3.513026 0.507762	H 0.347618 3.534263 0.448601
H 1.930310 3.280701 -0.258915	H 1.946163 3.316116 -0.319479
H -0.429550 -3.656664 0.513714	H -0.435246 -3.677163 0.452638
H -1.943397 -3.433702 -0.391856	H -1.958724 -3.464914 -0.455999
H 0.929891 -3.058926 -1.375362	H 0.919750 -3.051425 -1.403973
H -0.350778 -4.090112 -2.015143	H -0.345953 -4.089724 -2.068740
H -0.845874 2.896678 -1.486588	H -0.836414 2.878065 -1.513703
H 0.487932 3.919371 -2.022839	H 0.478763 3.915449 -2.076674
H -0.561420 -2.412637 -3.608164	H -0.577096 -2.400006 -3.650805
H -1.554076 -1.629023 -2.381946	H -1.559299 -1.620679 -2.410901
H 0.831492 2.223983 -3.573684	H 0.868126 2.208226 -3.606949

H 1.714723 1.454761 -2.257942	H 1.725735 1.442840 -2.269754
H 1.145757 -0.849672 -3.445915	H 1.154771 -0.858982 -3.467549
H 1.075898 -0.795221 -1.688294	H 1.063328 -0.804013 -1.709327
H -0.885177 0.662971 -3.540086	H -0.874489 0.668749 -3.574523
H -0.964532 0.627005 -1.782426	H -0.953373 0.633742 -1.815066

6	
S_0	S_1
51	51
FINAL HEAT OF FORMATION = -1147.438440	FINAL HEAT OF FORMATION = -1147.349950
C 3.319552 1.924482 0.429760	C 3.401648 1.949736 0.591097
C 2.084020 1.243811 0.492016	C 2.128234 1.290170 0.583505
N 2.374818 -0.116404 0.482725	N 2.398733 -0.089487 0.554623
C 3.740507 -0.314343 0.418264	C 3.756778 -0.303582 0.551577
C 4.345095 0.942786 0.387938	C 4.392481 0.952381 0.584611
C 0.731820 1.700281 0.576746	C 0.813929 1.749123 0.553776
C -0.293863 0.745111 0.646666	C -0.269733 0.740498 0.587781
C 0.003966 -0.680202 0.473641	C 0.023418 -0.647352 0.381074
C 1.406705 -1.156784 0.460195	C 1.425384 -1.113547 0.399597
C -1.020629 -1.607495 0.231182	C -1.014346 -1.635066 0.179751
C -2.374757 -1.150140 0.281530	C -2.337916 -1.183628 0.276486
N -2.660911 0.170897 0.612683	N -2.607583 0.153237 0.603459
C -1.695637 1.184939 0.860438	C -1.627458 1.178746 0.804104
C -3.619727 -1.790831 0.078220	C -3.617429 -1.825785 0.116452
C -4.638921 -0.828071 0.299465	C -4.598367 -0.858190 0.361207
C -4.026054 0.379675 0.632450	C -3.956600 0.365612 0.662313
O -2.093404 2.290492 1.209098	O -2.049627 2.310728 1.102329
C -0.832314 -3.058994 -0.154973	C -0.811297 -3.082202 -0.203639
C -0.346079 -3.281382 -1.613018	C -0.386026 -3.310056 -1.682131
C -0.931537 -2.310945 -2.663585	C -1.003611 -2.316966 -2.688872
C -0.067668 -1.037321 -2.861160	C -0.140679 -1.041066 -2.855493
C -0.795629 0.298786 -2.662364	C -0.869712 0.297774 -2.688012
C 0.190535 1.463086 -2.507115	C 0.126784 1.448825 -2.505597
O 1.791482 -2.320001 0.421721	O 1.808695 -2.280849 0.305859
C 0.529885 3.186900 0.401114	C 0.573847 3.217528 0.335151
H 4.142496 -1.325285 0.396272	H 4.147167 -1.319879 0.513370
H -4.421169 1.363799 0.876114	H -4.339192 1.356064 0.904166
H 5.419453 1.123517 0.340549	H 5.472911 1.103329 0.600403
H 3.447431 3.007012 0.427892	H 3.550257 3.029617 0.626766
H -5.714739 -0.989506 0.224497	H -5.679818 -1.000513 0.324451
H -3.763368 -2.835749 -0.194629	H -3.774715 -2.873583 -0.137902
H -0.127956 -3.547138 0.533912	H -0.073169 -3.561494 0.456002
H -1.807644 -3.555965 -0.035477	H -1.775397 -3.592308 -0.042224
H 0.755299 -3.222364 -1.641686	H 0.714860 -3.257839 -1.751917
H -0.607038 -4.323422 -1.873556	H -0.669034 -4.347205 -1.940697
H -1.020828 -2.845852 -3.625412	H -1.118924 -2.818320 -3.666139
H -1.962521 -2.027989 -2.377658	H -2.026200 -2.044355 -2.363233
H 0.401639 -1.049670 -3.863150	H 0.373856 -1.057658 -3.835581
H 0.774531 -1.066580 -2.145203	H 0.671272 -1.066386 -2.104945
H -1.501929 0.486877 -3.494130	H -1.545513 0.488796 -3.543991
H -1.409928 0.236082 -1.746396	H -1.511515 0.245003 -1.789871

C	-0.430612	2.771432	-1.975370	C	-0.480790	2.771938	-2.002204
H	0.983752	1.133357	-1.813250	H	0.889158	1.109934	-1.780666
H	0.704897	1.658370	-3.468072	H	0.678696	1.629243	-3.449005
C	0.541549	3.589145	-1.101403	C	0.520070	3.598951	-1.173479
H	-0.772596	3.390480	-2.824570	H	-0.829089	3.369788	-2.864282
H	-1.338548	2.545881	-1.384980	H	-1.377845	2.575134	-1.386221
H	1.342528	3.723732	0.920494	H	1.393115	3.788713	0.807063
H	-0.417599	3.498597	0.852558	H	-0.373124	3.509824	0.808293
H	0.284993	4.663417	-1.145253	H	0.260841	4.672962	-1.219147
H	1.566534	3.489748	-1.506733	H	1.532460	3.493918	-1.611020