Optimized Stuctures of Cyclohexynes (B3LYP/6-31G(d))

Cyclohexyne

0 1

C 0	1.590805	-0.198196	-0.116119
C 0	0.720627	1.054596	0.282059
C 0	-0.720627	1.054596	-0.282059
C 0	-1.590805	-0.198196	0.116119
C 0	-0.610077	-1.302063	0.021606
C 0	0.610077	-1.302063	-0.021606
H 0	1.983292	-0.103607	-1.136871
H 0	2.454956	-0.285614	0.552750
H 0	1.235245	1.964859	-0.053391
H 0	0.676117	1.098373	1.377808
H 0	-0.676117	1.098373	-1.377808
H 0	-1.235245	1.964859	0.053391
H 0	-1.983292	-0.103607	1.136871
H 0	-2.454956	-0.285614	-0.552750

4-Methylcyclohexyne

0 1

C 0	1.663330	-0.966644	-0.102600
C 0	0.140503	-1.158478	0.247284
C 0	-0.823318	-0.090988	-0.338074
C 0	-0.465134	1.389923	0.090790
C 0	1.010483	1.400421	0.042709
C 0	1.833847	0.500092	0.011078
C 0	-2.282425	-0.401337	0.025024
H 0	1.884232	-1.312256	-1.120789
H 0	2.285919	-1.559280	0.577896
H 0	0.040848	-1.159943	1.341248
H 0	-0.178192	-2.150009	-0.101395
H 0	-0.723602	-0.122009	-1.432678
H 0	-0.833572	1.603073	1.103622
H 0	-0.960083	2.098434	-0.584686
H 0	-2.958389	0.360748	-0.380768
H 0	-2.421249	-0.424896	1.113449
H 0	-2.599655	-1.371826	-0.373108

4-Ethylcyclohexyne

0 1

C 0	2.463547	-1.494339	-0.160660
C 0	1.000702	-1.158554	0.313339
C 0	0.375275	0.128036	-0.291855
C 0	1.233292	1.432175	-0.020721

C 0	2.621933	0.957321	-0.172134
C 0	3.109619	-0.161545	-0.182983
C 0	-1.068527	0.362732	0.196060
C 0	-2.100250	-0.652542	-0.311203
H 0	2.463531	-1.949158	-1.159729
H 0	2.923248	-2.220367	0.520157
H 0	1.012985	-1.059600	1.407440
H 0	0.359314	-2.017136	0.079208
H 0	0.351196	0.002869	-1.384872
H 0	1.049911	1.816605	0.992020
H 0	0.930450	2.220383	-0.720825
H 0	-1.077300	0.380081	1.295624
H 0	-1.380569	1.366684	-0.124573
H 0	-3.109619	-0.377762	0.015762
H 0	-2.106461	-0.694641	-1.407425
H 0	-1.899704	-1.663651	0.059341

4-*t*-Butylcyclohexyne

0 1

C 0	2.472214	-1.109268	-0.156265
C 0	0.959076	-1.098068	0.267120
C 0	0.106354	0.067230	-0.320724
C 0	0.671600	1.500473	0.076828
C 0	2.130844	1.309097	0.000809
C 0	2.846008	0.322479	-0.059082
C 0	-1.430100	-0.069733	-0.024734
C 0	-1.730316	-0.180161	1.484573
C 0	-1.991409	-1.321411	-0.736206
C 0	-2.182129	1.155136	-0.591385
H 0	2.598846	-1.479202	-1.182144
H 0	3.040970	-1.781464	0.497070
H 0	0.924606	-1.053909	1.362381
H 0	0.519882	-2.057816	-0.027252
H 0	0.210938	0.014862	-1.415054
H 0	0.359604	1.795395	1.086792
H 0	0.283173	2.257385	-0.611908
H 0	-2.813766	-0.214142	1.651108
H 0	-1.341171	0.677124	2.045883
H 0	-1.304153	-1.089325	1.921890
H 0	-3.080078	-1.371643	-0.612381
H 0	-1.576019	-2.251358	-0.334854
H 0	-1.780838	-1.294357	-1.812637
H 0	-3.265030	1.005295	-0.507889
H 0	-1.950165	1.310715	-1.652649
H 0	-1.939621	2.077759	-0.053909

4-Phenylcylcohexyne

	0	1		
C	0	-3.058105	0.676834	0.990600
C	0	-1.510452	0.410767	1.082275
C	0	-0.770889	0.313812	-0.287186
C	0	-1.348755	-0.816223	-1.246002
C	0	-2.804276	-0.710220	-1.028015
C	0	-3.463058	-0.174332	-0.151428
C	0	0.730652	0.152557	-0.111435
C	0	1.276917	-0.971161	0.528366
C	0	2.656128	-1.112030	0.678696
C	0	3.520935	-0.131317	0.187836
C	0	2.993195	0.989471	-0.453308
C	0	1.611511	1.126663	-0.599716
H	0	-3.270203	1.734955	0.790237
H	0	-3.538788	0.429962	1.944443
H	0	-1.356140	-0.521072	1.640076
H	0	-1.045303	1.212509	1.669464
H	0	-0.946671	1.262177	-0.811615
H	0	-0.971420	-1.806442	-0.963028
H	0	-1.009811	-0.627716	-2.271225
H	0	0.618912	-1.745132	0.916443
H	0	3.056213	-1.990097	1.179214
H	0	4.595764	-0.241531	0.303864
H	0	3.655472	1.759338	-0.840897
H	0	1.208969	2.004196	-1.101181

3-Methylcyclohexyne

	0	1		
C	0	2.019089	-0.321335	0.275528
C	0	1.321609	1.006363	-0.210052
C	0	-0.180725	1.114334	0.140564
C	0	-1.098892	-0.045593	-0.415710
C	0	-0.223465	-1.227707	-0.202774
C	0	0.974533	-1.334839	0.009460
C	0	-2.470566	-0.069351	0.265900
H	0	2.263565	-0.275284	1.344696
H	0	2.961929	-0.473175	-0.262726
H	0	1.441071	1.070572	-1.299179
H	0	1.852997	1.865906	0.220139
H	0	-0.566971	2.072418	-0.234222
H	0	-0.294983	1.130707	1.232986
H	0	-1.248856	0.101242	-1.494919
H	0	-2.991943	0.883896	0.117661
H	0	-2.368561	-0.240173	1.343338
H	0	-3.097702	-0.867233	-0.145279

4-Cyanocyclohexyne

	0	1		
C	0	-1.836868	-1.095078	0.076218
C	0	-0.294266	-1.159744	-0.229263
C	0	0.531158	0.017303	0.384125
C	0	0.070770	1.469467	-0.084839
C	0	-1.398712	1.338684	-0.082993
C	0	-2.111679	0.349960	-0.044556
C	0	1.958969	-0.163467	0.100388
N	0	3.088593	-0.283447	-0.141769
H	0	-2.062988	-1.465363	1.083786
H	0	-2.378540	-1.731888	-0.631882
H	0	-0.151321	-1.155853	-1.315506
H	0	0.111435	-2.105392	0.148865
H	0	0.404846	-0.012863	1.474442
H	0	0.459579	1.695984	-1.084213
H	0	0.480560	2.216888	0.602417