Isolation, X-ray crystallography, and Computational Studies of Calydaphninone, a Novel Alkaloid from *Daphniphyllum calycillum*

Ying-Tong Di,^[a,c] Hong-Ping He,^[a] Yun-Song Wang,^[d] Liang-Bo Li,^[a] Yang Lu,^[b] Ning-Bo Gong,^[b] Xin Fang,^[a] Ning-Chuan Kong,^[a] Shun-Lin Li,^[a] Hua-Jie Zhu,^{*,[a]} Xiao-Jiang Hao^{*,[a]}

State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650204, Yunnan, PR China, Institute of Materia Medica, Chinese Academy of Medical Sciences, Beijing 100050, P. R. China, Graduate School of the Chinese Academy of Sciences, Beijing 100039, PR China, and Key Laboratory of Medicinal Chemistry for Natural Resources, Ministry of Education, Research School of Pharmacy, Yunnan University, Kunming, Yunnan 650091, PRC

* Corresponding author, Phone: (+86) 871-5223263, Fax: (+86) 871-5219684. Email address: haoxj@mail.kib.ac.cn, hjzhu@mail.kib.ac.cn

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Experimental Section

General Experimental Procedures. Optical rotation was carried out on a Perkin-Elmer model 241 polarimeter. IR spectrum was measured in a Bio-Rad FTS-135 spectrometer with KBr pellets. ESI and high-resolution mass spectra were recorded using a Finnigan MAT 90 instrument and VG Auto Spec-3000 spectrometer respectively. ^1H and 2D NMR spectra were measured on a Bruker DRX-500 instrument, while ^{13}C NMR spectra were recorded on a Bruker AM-400 spectrometer. Chemical shifts were reported using residual CDCl_3 (δ_{H} 7.26 and δ_{C} 77.0) as internal standard. Column chromatography was performed on silica gel H (10–40 μm ; Qingdao Marine Chemical Inc.), amino silica gel (75–100 μm , Fuji Silysia Chemical LTD, Japan), Precoated silica gel GF254 and HF254 plates (Qingdao Haiyang Chemical Plant, Qingdao, People's Republic of China) were used for TLC.

Plant Material. The leaves and twigs of *Daphniphyllum calycillum* Benth were collected in Xishuangbanna of Yunnan Province, People's Republic of China, in August, 2004. The sample was identified by Prof. De-Ding Tao, Kunming Institute of Botany, Chinese Academy Sciences, and a voucher specimen (KIB 04100537) deposited at the State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy Sciences.

Extraction and isolation. The air-dried and powdered leaves and stems of the plant (7 Kg) were extracted with 95% EtOH at 333 K for 12 hour. Evaporation of the solvent (under vacuum, 333 K) gave a residue, which was suspended in water (2 L) and adjusted to pH 3 with saturated tartaric acid. The acidic mixture was defatted with EtOAc (3×2 L), and then aqueous layer was then basified to pH 10 with 2N NaOH, followed by exhaustive extraction with CHCl_3 (3×2 L) to yield the crude alkaloids (15 g). The crude alkaloids were separated by an amino silica gel column chromatography, using $\text{CHCl}_3/\text{MeOH}$ (1:0 $\rightarrow$ 0:1) as eluent, to give nine fractions. The fraction, eluted with $\text{CHCl}_3/\text{MeOH}$ (20:1), was chromatographed on normal H silica gel ($\text{CHCl}_3/\text{MeOH}$, 50:1 $\rightarrow$ 20:1) to afford **1** (6 mg).

X-ray crystal structure of Calydaphninone (1): colorless block crystal of **1** were obtained by recrystallization in acetone. The crystal belongs to orthorhombic formula $\text{C}_{23}\text{H}_{31}\text{NO}_4$ ($M_r = 385.49$), space group $\text{P2}_1\text{2}_1\text{2}_1$, $a = 6.480$ (1), $b = 14.678$ (1), $c = 21.037$ (1) Å; $\alpha = \beta = \gamma = 90.0^\circ$; $V = 2009.2$ (2)

$\text{\AA}^3$; $Z = 4$; and $\rho_{\text{calcd}} = 1.280 \text{ mgmm}^{-3}$, a crystal of dimensions $0.05 \times 0.10 \times 0.30 \text{ mm}$, was used for measurements on a MAC DIP-2030K diffractometer with a graphite monochromator (ω - 2θ scans, $2\theta_{\text{MAX}} = 50.0^\circ$), Mo KR radiation. The total number of independent reflections measured was 2374, of which 2305 were observed ($|F|^2 \geq 2\sigma|F|^2$). The crystal structure of **1** was solved by direct methods using SHELXS-97 (Sheldrich, G. M. University of Gottingen: Gottingen, Germany, 1997) and expanded using difference Fourier techniques, refined by the program and method SHELXS-97 and full-matrix least-squares calculations. All non-hydrogen atoms were given anisotropic thermal parameters. The hydrogen atom positions were geometrically idealized and allowed to ride on their parent atoms. The final indices were $R_1 = 0.056$, $wR_2 = 0.161$.

Computational method: The Gaussian 03 package was used in the computations of different conformations and transition states (TS). Hartree-Fork (HF) theory was applied to search for the low energy conformations at the 3-21G* level, using the crystal as original geometry. The obtained geometries were further optimized at the B3LYP/6-31G* level of theory in the gas phase. The TS geometries were directly obtained at the B3LYP/6-31G* level using the lowest energy conformations. Only one negative eigenvalue and one imaginary frequency were obtained for each TS in computations. Frequency analyses confirmed that the calculated TS structures were the expected geometries. The free energy magnitudes were used throughout the theoretical studies.

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Table S1: ^1H and ^{13}C NMR data of calydaphninone in CDCl_3

No.	^{13}C NMR	^1H NMR	HMBC
1	213.5		
2	74.5 ^a		
3 α	35.4	1.93 (1H, m)	1, 2 (4), 5, 18
3 β		2.25 (1H, m)	1, 2 (4), 5, 18
4	74.5 ^a	3.89 (1H, br d, 9.0)	2, 5, 6, 21
5	44.9		
6	38.4	2.64 (1H, m)	
7	55.7	2.63 (1H, m) 2.80 (1H, m)	2, 5, 6 5,6
8	58.7		
9	142.0		
10	134.2		
11	25.8	3.03 (1H, m) 1.81 (1H, m)	6, 9
12 α	26.0	1.63 (1H, m)	5, 6, 7, 11
12 β		2.03 (1H, m)	
13 α	39.5	1.83 (1H, m)	1, 8, 9, 14, 15, 22
13 β		2.73 (1H, m)	1, 5, 8, 14, 15, 22
14	42.0	3.04 (1H, m)	8, 9, 13, 15, 22
15	56.2	3.98 (1H, m)	
16 α	29.2	1.94 (1H, m)	9, 11, 10, 15, 17
16 β		1.24 (1H, m)	15, 17
17	42.6	2.61 (1H, m) 2.28 (1H, m)	9, 10 9, 10, 15, 16
18	25.7	2.95 (1H, m)	1, 2, 19, 20
19	57.7	3.02 (1H, m) 2.97 (1H, m)	7, 18, 20 7, 18, 20
20	14.8	1.12 (3H, d, 7.0)	2, 18, 19
21	24.4	1.33 (3H, s)	4, 5, 6, 8
22	175.6		
23	51.3	3.65 (3H, m)	22

^a overlapped

Figure S1. Key NOESY ($\curvearrowright$) correlations of calydaphninone in CDCl_3 1.

Table S2: ^1H and ^{13}C NMR data for TFA salt of calydaphninone in CDCl_3

	3^a		4^a	
	δ_{C}	δ_{H}	δ_{C}	δ_{H}
1	205.0		203.6	
2	77.0 ^b		78.6	
3	32.9	2.77 (1H, m) 2.19 (1H, m)	31.0	2.98 (1H, m) 2.38 (1H, m)
4	77.0 ^b	5.18 (br d, 9.5)	71.8	4.19 (1H, d, 9.5)
5	44.9		44.4	
6	35.4	3.00 (1H, m)	36.8	2.96 (1H, m)
7 α	54.1	3.47 (1H, m)	53.4	3.70 (1H, m)
7 β		3.06 (1H, m)		3.07 (1H, m)
8	59.1		59.0	
9	140.3		139.4	
10	135.6		136.4	
11 α	23.9	2.19 (1H, m)	24.0	2.21 (1H, m)
11 β		1.76 (1H, m)		1.71 (1H, m)
12 α	24.8	2.29 (1H, m)	24.8	2.30 (1H, m)
12 β		2.10 (1H, m)		2.09 (1H, m)
13 β	40.0	2.87 (1H, m)	39.7	2.85 (1H, m)
13 α		1.92 (1H, m)		1.96 (1H, m)
14	42.0	3.23 (1H, m)	41.9	3.20 (1H, m)
15	56.0	4.04 (1H, m)	55.9	4.02 (1H, m)
16 α	29.1	2.04 (1H, m)	29.2	2.06 (1H, m)
16 β		1.30 (1H, m)		1.30 (1H, m)
17 α	42.9	2.68 (1H, m)	42.8	2.66 (1H, m)
17 β		2.38 (1H, m)		2.37 (1H, m)
18	26.8	3.42 (1H, m)	27.0	3.44 (1H, m)
19 β	58.7	3.86 (1H, m)	58.9	3.87 (1H, m)
19 α		3.71 (1H, m)		3.74 (1H, m)
20	12.8	1.30 (3H, d, 7.5)	12.3	1.31 (3H, d, 7.5)
21	23.5	1.36 (3H, s)	23.1	1.39 (3H, s)
22	176.5		176.2	
23	52.3	3.73 (3H, s)	52.3	3.73 (3H, s)
NH				

^a Assignment of NMR data based on comparison of 1D and 2D NMR spectra before and after the solution was heated, which was consistent with computational results.

^b overlapped with CDCl₃

Figure S2. ¹H,¹H COSY (—) and selected HMBC (⤿) correlations of 2.

Figure S3. Key NOESY (⤿) correlations of 1.

Figure S4. DFT-calculated conformations of HCl salt of **1**, a model of its TFA salt. Energies (in italic, KJmol⁻¹) relative to the stablest conformer BHC-HCl.

^{13}C NMR spectrum of Calydaphninone (**1**) in CDCl_3 at 298 K

¹H-¹H COSY spectrum of Calydaphninone (**1**) in a mixture of CDCl₃ at 298 K

HMQC spectrum of Calydaphninone (**1**) in a mixture of CDCl_3 at 298 K

HMBC spectrum of Calydaphninone (**1**) in a mixture of CDCl_3 at 298 K

ROESY spectrum of Calydaphninone (**1**) in a mixture of CDCl_3 at 298 K

^{13}C NMR spectrum of Calydaphninone (**1**) in a mixture of CDCl_3 and Py-D_5 (3:1) at 298 K

^1H - ^1H COSY spectrum of Calydaphninone (**1**) in a mixture of CDCl_3 and Py-D_5 (3:1) at 298 K

TOCSY spectrum of Calydaphninone (**1**) in a mixture of CDCl_3 and Py-D_5 (3:1) at 298 K

HMQC spectrum of Calydaphninone (**1**) in a mixture of CDCl_3 and Py-D_5 (3:1) at 298 K

HMBC spectrum of Calydaphninone (**1**) in a mixture of CDCl_3 and Py-D_5 (3:1) at 298 K

NOESY spectrum of Calydaphninone (**1**) in a mixture of CDCl_3 and Py-D_5 (3:1) at 298 K

^1H NMR spectrum of Calydaphninone (**1**) in a mixture of CDCl_3 and Py-D_5 (3:1) at 333 K

^{13}C NMR spectrum of Calydaphninone (**1**) in a mixture of CDCl_3 and Py-D_5 (3:1) at 333 K

^{13}C NMR spectrum of TFA salt form of Calydaphninone in CDCl_3 at 298 K, recorded after TFA was added

^1H NMR spectrum of TFA salt of Calydaphninone in CDCl_3 at 298 K, recorded after the solution was heated to 333 K for 20 min

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ROESY spectrum of TFA salt of Calydaphninone in CDCl_3 at 298 K, recorded after the solution was heated to 333 K for 20 min

All conformations and transition state structures were obtained at the B3LYP/6-31G(d) level of theory. Only one negative eigenvalue and one imaginary frequency were obtained in the TS computations. Eigenvalue and frequency analyses confirmed that the calculated TS structures were the expected geometries. The free energy magnitudes were used throughout the theoretical studies.

Conformation CTC:

Free energy = -1250.237018 a.u.

(hydrogen atoms were hidden for clarity)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.826027	-0.884942	-0.798337
2	6	0	-1.080164	2.209219	-0.903244
3	6	0	-0.037824	3.260048	-0.653663
4	6	0	1.389846	2.695690	-0.649506
5	6	0	-1.090502	-0.954835	0.780008
6	6	0	-2.280332	-1.102730	-0.200818
7	6	0	-2.182605	0.129655	-1.167907
8	6	0	-3.262272	1.232651	-1.226813
9	6	0	-2.436934	2.513776	-1.524338
10	6	0	3.197902	-1.895963	-1.326507
11	6	0	4.146957	-0.669756	-1.331586
12	6	0	2.287784	-1.046838	-0.390198
13	6	0	3.730789	-3.248736	-0.878905
14	6	0	-0.020143	1.560531	2.191839
15	6	0	-3.607711	-1.161338	0.527895
16	6	0	-5.870110	-1.797497	0.329162
17	6	0	2.385779	-1.336336	1.114650
18	6	0	1.615787	-0.317336	1.990473

19	6	0	0.861652	0.787993	1.174736
20	6	0	1.881689	1.832100	0.542880
21	6	0	3.240241	1.225340	0.121116
22	6	0	-0.031676	0.024518	0.118005
23	6	0	-0.970409	0.892247	-0.686985
24	1	0	-0.251330	3.821274	0.270260
25	1	0	-0.104217	4.007280	-1.458027
26	1	0	2.092582	3.536778	-0.723063
27	1	0	1.518873	2.110618	-1.567547
28	1	0	-0.661423	-1.929735	1.035150
29	1	0	-1.469921	-0.511241	1.701212
30	1	0	-2.186573	-2.013410	-0.795026
31	1	0	-1.999142	-0.259481	-2.176660
32	1	0	-4.043919	1.039832	-1.968838
33	1	0	-3.743753	1.339088	-0.247019
34	1	0	-2.342804	2.686199	-2.608595
35	1	0	-2.894393	3.420749	-1.106819
36	1	0	2.691937	-1.993228	-2.290808
37	1	0	4.964298	-0.776413	-0.597159
38	1	0	4.574728	-0.349094	-2.289342
39	1	0	2.923794	-3.987277	-0.803861
40	1	0	4.236007	-3.198389	0.092228
41	1	0	4.456069	-3.630214	-1.607889
42	1	0	-0.592139	0.887044	2.837993
43	1	0	-0.737137	2.221354	1.703826
44	1	0	0.606039	2.182817	2.841685
45	1	0	-6.492165	-2.298390	-0.413349
46	1	0	-6.245111	-0.789690	0.527354
47	1	0	-5.860555	-2.361252	1.265914
48	1	0	2.046095	0.715037	3.596913
49	1	0	3.431666	-1.334223	1.436439
50	1	0	2.008373	-2.348538	1.304277
51	1	0	0.846347	-0.863766	2.553248
52	1	0	2.119205	2.516786	1.366083
53	1	0	3.841820	2.008203	-0.359527
54	1	0	3.796747	0.891736	1.009385
55	7	0	3.032580	0.164665	-0.845780
56	8	0	0.351750	-1.453573	-1.765027
57	8	0	2.550348	0.221761	2.931855
58	8	0	-3.838582	-0.720261	1.636149
59	8	0	-4.553604	-1.745163	-0.242942

Conformation CC:

Free energy = -1250.237029 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.982842	-0.058561	-1.313665
2	6	0	-0.850516	2.008051	0.720000
3	6	0	0.127982	2.368355	1.797435
4	6	0	0.537040	1.187902	2.688589
5	6	0	-1.124654	-1.340604	-0.870023
6	6	0	-2.386313	-0.523977	-1.281731
7	6	0	-1.970931	0.968043	-1.089570
8	6	0	-2.923434	2.045330	-0.533012
9	6	0	-1.983845	2.942156	0.315725
10	6	0	3.480403	0.541755	-1.819855
11	6	0	3.934055	1.358686	-0.584222
12	6	0	2.430922	-0.106480	-0.870809
13	6	0	4.503977	-0.320246	-2.544134
14	6	0	-0.439875	-1.629991	2.001333
15	6	0	-3.594843	-0.874765	-0.437077
16	6	0	-5.954376	-0.893903	-0.392940
17	6	0	2.708897	-1.532172	-0.366567
18	6	0	1.620232	-2.043423	0.609168
19	6	0	0.624903	-0.939452	1.104158
20	6	0	1.394849	0.075248	2.044101
21	6	0	2.737331	0.629134	1.513216
22	6	0	-0.064254	-0.357884	-0.204137
23	6	0	-0.870043	0.917368	-0.057879
24	1	0	-0.308983	3.148364	2.435231
25	1	0	1.022506	2.814100	1.338122
26	1	0	-0.365836	0.752710	3.132165

27	1	0	1.122539	1.586553	3.528732
28	1	0	-0.693238	-1.811826	-1.755407
29	1	0	-1.414493	-2.130058	-0.180327
30	1	0	-2.656374	-0.709222	-2.324029
31	1	0	-1.550337	1.296333	-2.049430
32	1	0	-3.459942	2.596326	-1.311707
33	1	0	-3.670766	1.593029	0.128786
34	1	0	-1.594514	3.785014	-0.277926
35	1	0	-2.489594	3.385864	1.183605
36	1	0	2.952759	1.173698	-2.539540
37	1	0	4.831133	0.926119	-0.108499
38	1	0	4.087651	2.437596	-0.706052
39	1	0	4.026091	-0.940077	-3.311573
40	1	0	5.045958	-0.983364	-1.860337
41	1	0	5.245167	0.312439	-3.047294
42	1	0	-0.696015	-2.631250	1.636999
43	1	0	-1.374991	-1.067565	2.040498
44	1	0	-0.072660	-1.743691	3.027539
45	1	0	-6.763545	-0.670200	-1.088830
46	1	0	-6.014974	-0.246926	0.486505
47	1	0	-6.003988	-1.936599	-0.068002
48	1	0	1.647862	-3.137162	2.229347
49	1	0	3.676337	-1.583324	0.141407
50	1	0	2.776780	-2.204161	-1.229636
51	1	0	1.008536	-2.792990	0.082820
52	1	0	1.696110	-0.563991	2.882174
53	1	0	3.007356	1.526629	2.085214
54	1	0	3.533964	-0.109778	1.710136
55	7	0	2.681613	0.993364	0.111713
56	8	0	0.658369	0.166944	-2.465976
57	8	0	2.310417	-2.687341	1.681552
58	8	0	-3.583264	-1.274814	0.710248
59	8	0	-4.741009	-0.648481	-1.120986

Conformation BHC:

Free energy = -1250.236696 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.888717	-0.983622	-0.671055
2	6	0	-0.964022	2.103272	-0.955283
3	6	0	0.020205	3.232872	-0.792086
4	6	0	1.082099	3.149553	0.326342
5	6	0	-1.092331	-1.032490	0.856755
6	6	0	-2.250995	-1.174079	-0.163762
7	6	0	-2.071315	0.017311	-1.168293
8	6	0	-3.132822	1.115057	-1.371236
9	6	0	-2.266555	2.352599	-1.714710
10	6	0	3.197634	-1.946893	-1.289822
11	6	0	3.613943	-0.577546	-1.891395
12	6	0	2.367517	-1.117976	-0.262492
13	6	0	4.345574	-2.785415	-0.737806
14	6	0	-0.027239	1.407538	2.325397
15	6	0	-3.606077	-1.151526	0.515260
16	6	0	-5.879906	-1.724992	0.261875
17	6	0	2.461778	-1.396179	1.230572
18	6	0	1.709282	-0.348443	2.077890
19	6	0	0.860689	0.701972	1.267441
20	6	0	1.774327	1.784091	0.560766
21	6	0	2.433817	1.355957	-0.766884
22	6	0	-0.005484	-0.077283	0.224639
23	6	0	-0.887265	0.799228	-0.639904
24	1	0	-0.540660	4.168427	-0.655114
25	1	0	0.524434	3.358530	-1.763494
26	1	0	0.642182	3.505345	1.260542

27	1	0	1.867270	3.878078	0.082932
28	1	0	-0.681444	-2.008209	1.138106
29	1	0	-1.495518	-0.571871	1.759671
30	1	0	-2.174557	-2.110360	-0.719514
31	1	0	-1.809963	-0.417418	-2.140779
32	1	0	-3.871246	0.874149	-2.142730
33	1	0	-3.668171	1.301377	-0.432064
34	1	0	-2.081266	2.415756	-2.799379
35	1	0	-2.739171	3.300629	-1.426206
36	1	0	2.559933	-2.542450	-1.946183
37	1	0	4.680825	-0.422932	-2.097528
38	1	0	3.034281	-0.313566	-2.790784
39	1	0	3.980465	-3.627101	-0.137305
40	1	0	5.019451	-2.188724	-0.113134
41	1	0	4.937032	-3.201021	-1.562495
42	1	0	-0.468339	0.689126	3.023382
43	1	0	-0.848471	1.967248	1.873267
44	1	0	0.563520	2.114878	2.920424
45	1	0	-6.490793	-2.243027	-0.478139
46	1	0	-6.228728	-0.697454	0.396292
47	1	0	-5.922491	-2.241150	1.224751
48	1	0	2.196619	0.798857	3.585154
49	1	0	3.512724	-1.375085	1.528888
50	1	0	2.075378	-2.400560	1.448380
51	1	0	0.985350	-0.884828	2.708441
52	1	0	2.587503	1.962576	1.273906
53	1	0	1.680813	1.330510	-1.576696
54	1	0	3.161451	2.128659	-1.049935
55	7	0	3.140210	0.094082	-0.662824
56	8	0	0.428461	-1.558092	-1.642996
57	8	0	2.676520	0.269610	2.928995
58	8	0	-3.862422	-0.647294	1.590265
59	8	0	-4.542472	-1.742350	-0.262032

Transition state structure TS1 (CTC-CC):

Free energy = -1250.220590 a.u.

Frequency: -183.773 .

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.768121	-1.208280	-0.393752
2	6	0	-0.958186	1.899015	-1.233305
3	6	0	-0.176389	3.145207	-0.957391
4	6	0	1.240303	3.117492	-0.323214
5	6	0	-1.174091	-0.753482	1.093588
6	6	0	-2.285399	-1.129232	0.080021
7	6	0	-2.025357	-0.222159	-1.179970
8	6	0	-3.070584	0.808823	-1.656737
9	6	0	-2.208935	2.015467	-2.099070
10	6	0	3.094708	-2.056665	-1.222424
11	6	0	3.765626	-0.759974	-1.739938
12	6	0	2.273726	-1.127922	-0.280585
13	6	0	3.973721	-3.158578	-0.649516
14	6	0	0.085042	1.740988	2.129543
15	6	0	-3.668990	-0.927869	0.663067
16	6	0	-5.944113	-1.502981	0.423933
17	6	0	2.666280	-1.081599	1.202732
18	6	0	1.799632	-0.097941	2.025009
19	6	0	0.930016	0.877241	1.156510
20	6	0	1.883531	1.884469	0.400656
21	6	0	3.046597	1.253850	-0.413700
22	6	0	-0.016153	-0.045589	0.280938
23	6	0	-0.854913	0.650408	-0.763310
24	1	0	-0.830129	3.770330	-0.327109

25	1	0	-0.107279	3.710593	-1.898154
26	1	0	1.260372	3.951098	0.388273
27	1	0	1.949756	3.408899	-1.104216
28	1	0	-0.823969	-1.631010	1.647488
29	1	0	-1.602466	-0.052915	1.810698
30	1	0	-2.200478	-2.172464	-0.223598
31	1	0	-1.745555	-0.885318	-2.006185
32	1	0	-3.725906	0.428590	-2.447040
33	1	0	-3.703588	1.120788	-0.817533
34	1	0	-1.946743	1.955738	-3.167097
35	1	0	-2.722667	2.976477	-1.960378
36	1	0	2.416466	-2.475982	-1.970458
37	1	0	4.752247	-0.589925	-1.274304
38	1	0	3.861172	-0.624186	-2.823919
39	1	0	3.368286	-3.958026	-0.206431
40	1	0	4.660578	-2.787171	0.119595
41	1	0	4.581103	-3.609944	-1.443492
42	1	0	-0.341349	1.146347	2.944582
43	1	0	-0.747153	2.232485	1.618914
44	1	0	0.700039	2.527075	2.582776
45	1	0	-6.534190	-2.165081	-0.210739
46	1	0	-6.268016	-0.465658	0.301737
47	1	0	-6.049828	-1.783856	1.475326
48	1	0	2.158994	1.072855	3.550717
49	1	0	3.714599	-0.789661	1.318105
50	1	0	2.579818	-2.089818	1.623796
51	1	0	1.087928	-0.681454	2.628167
52	1	0	2.420194	2.339519	1.240133
53	1	0	3.406408	1.976911	-1.155472
54	1	0	3.896015	1.082103	0.272961
55	7	0	2.691755	0.040844	-1.114804
56	8	0	0.208202	-2.121831	-0.973427
57	8	0	2.694257	0.583152	2.906858
58	8	0	-3.964331	-0.190458	1.582713
59	8	0	-4.584640	-1.664286	-0.008895

Transition state structure TS2 (CC-BHC):

Free energy = -1250.224111 a.u.

Frequency: -231.931

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.822713	-1.203229	-0.422208
2	6	0	-0.906961	1.964451	-1.127575
3	6	0	0.012461	3.148751	-0.988080
4	6	0	1.064482	3.167320	0.142058
5	6	0	-1.166838	-0.869611	1.040797
6	6	0	-2.275538	-1.154982	-0.002797
7	6	0	-2.012217	-0.138174	-1.170844
8	6	0	-3.047288	0.930586	-1.571109
9	6	0	-2.161044	2.128150	-1.985578
10	6	0	3.160780	-2.022293	-1.225178
11	6	0	3.607464	-0.705540	-1.932688
12	6	0	2.340580	-1.125260	-0.236295
13	6	0	4.264923	-2.910901	-0.669140
14	6	0	0.052200	1.536899	2.283099
15	6	0	-3.661464	-1.004978	0.591189
16	6	0	-5.933878	-1.568466	0.303837
17	6	0	2.740363	-1.091278	1.237191
18	6	0	1.803174	-0.202879	2.069296
19	6	0	0.906281	0.778324	1.233231
20	6	0	1.794788	1.842542	0.470765
21	6	0	2.578334	1.434082	-0.819409
22	6	0	-0.007280	-0.094167	0.300379
23	6	0	-0.834463	0.693239	-0.695708
24	1	0	-0.608034	4.050406	-0.879041
25	1	0	0.509384	3.286777	-1.960977

26	1	0	0.605233	3.569167	1.047695
27	1	0	1.831260	3.902392	-0.139431
28	1	0	-0.817392	-1.790854	1.518615
29	1	0	-1.596322	-0.233291	1.814657
30	1	0	-2.189643	-2.166718	-0.399745
31	1	0	-1.724049	-0.723404	-2.052459
32	1	0	-3.732432	0.601710	-2.359068
33	1	0	-3.646868	1.218987	-0.699257
34	1	0	-1.907556	2.083827	-3.057149
35	1	0	-2.650391	3.097823	-1.824213
36	1	0	2.475162	-2.608154	-1.841497
37	1	0	4.685113	-0.483501	-1.828482
38	1	0	3.344768	-0.618446	-2.999339
39	1	0	3.855970	-3.736166	-0.074424
40	1	0	4.965806	-2.353289	-0.037417
41	1	0	4.840756	-3.353206	-1.491079
42	1	0	-0.323928	0.857085	3.055211
43	1	0	-0.814477	2.030161	1.837256
44	1	0	0.647806	2.306105	2.786976
45	1	0	-6.520771	-2.178169	-0.384026
46	1	0	-6.262303	-0.526052	0.268412
47	1	0	-6.038364	-1.936542	1.328102
48	1	0	2.054911	0.873612	3.685443
49	1	0	3.755865	-0.689578	1.317539
50	1	0	2.758876	-2.103978	1.658017
51	1	0	1.099302	-0.851481	2.612742
52	1	0	2.548649	2.098192	1.224639
53	1	0	2.071413	1.859586	-1.698719
54	1	0	3.559447	1.941238	-0.771995
55	7	0	2.755525	0.028544	-1.021273
56	8	0	0.287528	-2.042879	-1.125936
57	8	0	2.631664	0.471878	3.017446
58	8	0	-3.960179	-0.344124	1.566087
59	8	0	-4.573424	-1.687321	-0.140031

Conformation CTC-HCl:

Free energy = -1711.043386 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.615684	-0.762481	-0.797525
2	6	0	-1.129431	2.299537	0.178402
3	6	0	-0.121594	3.079688	0.971689
4	6	0	1.294413	2.498548	0.877547
5	6	0	-1.471017	-1.237389	0.459402
6	6	0	-2.523246	-0.902022	-0.625557
7	6	0	-2.244871	0.589610	-1.031611
8	6	0	-3.268724	1.718013	-0.773544
9	6	0	-2.374970	2.936471	-0.420918
10	6	0	3.034096	-1.643120	-1.481599
11	6	0	4.081396	-0.696393	-0.842077
12	6	0	2.043759	-1.141186	-0.391808
13	6	0	3.347448	-3.123107	-1.626558
14	6	0	-0.445925	0.389926	2.828047
15	6	0	-3.935341	-1.112256	-0.116011
16	6	0	-6.179190	-1.414204	-0.776902
17	6	0	1.975235	-1.989979	0.882540
18	6	0	1.158202	-1.349788	2.031278
19	6	0	0.519502	0.030218	1.666098
20	6	0	1.630887	1.167274	1.606352
21	6	0	3.022316	0.702433	1.116738
22	6	0	-0.286153	-0.188766	0.322704
23	6	0	-1.081582	1.004796	-0.160087
24	1	0	-0.449643	3.199772	2.016651
25	1	0	-0.083153	4.100207	0.567019

26	1	0	2.000486	3.241028	1.273028
27	1	0	1.529919	2.414734	-0.189401
28	1	0	-1.129561	-2.275319	0.379763
29	1	0	-1.947360	-1.118057	1.433286
30	1	0	-2.389853	-1.530240	-1.507468
31	1	0	-1.945447	0.594505	-2.086567
32	1	0	-3.934616	1.902209	-1.622342
33	1	0	-3.889431	1.469699	0.096106
34	1	0	-2.114717	3.518216	-1.318460
35	1	0	-2.861896	3.634984	0.272417
36	1	0	2.714062	-1.220625	-2.438640
37	1	0	4.698809	-1.165342	-0.070689
38	1	0	4.671971	-0.059022	-1.501876
39	1	0	2.467945	-3.671489	-1.981301
40	1	0	3.680566	-3.576977	-0.686451
41	1	0	4.143262	-3.266857	-2.365897
42	1	0	-1.052984	-0.467998	3.133722
43	1	0	-1.136442	1.189401	2.558330
44	1	0	0.114965	0.723358	3.708549
45	1	0	-6.720562	-1.528586	-1.716392
46	1	0	-6.528202	-0.529729	-0.237276
47	1	0	-6.318692	-2.293911	-0.142923
48	1	0	1.488540	-1.064234	3.942122
49	1	0	2.977045	-2.217121	1.259495
50	1	0	1.532340	-2.952274	0.602622
51	1	0	0.327175	-2.025310	2.272431
52	1	0	1.811110	1.414642	2.658997
53	1	0	3.688655	1.565306	1.017986
54	1	0	3.466205	-0.005906	1.817659
55	7	0	2.942147	0.074210	-0.217961
56	8	0	0.201985	-1.030089	-1.906385
57	8	0	2.027389	-1.284147	3.166293
58	8	0	-4.284616	-1.108358	1.047999
59	8	0	-4.797271	-1.270429	-1.143953
60	1	0	2.722460	0.840321	-1.011757
61	17	0	2.748633	1.944140	-2.429308

Conformation CC-HCl:

Free energy = -1711.044527 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.734930	-0.266138	-1.276565
2	6	0	-0.879001	1.602383	1.206894
3	6	0	0.062000	1.705174	2.366955
4	6	0	0.526467	0.374283	2.963598
5	6	0	-1.453372	-1.388278	-0.870924
6	6	0	-2.548423	-0.357992	-1.275512
7	6	0	-2.003465	1.030986	-0.801470
8	6	0	-2.878955	2.067836	-0.070465
9	6	0	-1.888500	2.707832	0.934216
10	6	0	3.281601	0.217714	-1.847942
11	6	0	3.971697	0.693038	-0.547273
12	6	0	2.206868	-0.440920	-0.939078
13	6	0	4.068675	-0.612413	-2.848743
14	6	0	-0.647128	-2.176135	1.852769
15	6	0	-3.872906	-0.681480	-0.612996
16	6	0	-6.212279	-0.431755	-0.782037
17	6	0	2.407667	-1.926860	-0.614468
18	6	0	1.328255	-2.505979	0.332023
19	6	0	0.428546	-1.427383	1.017856
20	6	0	1.298709	-0.615154	2.061081
21	6	0	2.657589	-0.041222	1.576972
22	6	0	-0.270946	-0.613793	-0.150851
23	6	0	-0.950303	0.690089	0.226068
24	1	0	-0.424591	2.277181	3.168742
25	1	0	0.915654	2.321932	2.047438
26	1	0	-0.339715	-0.144821	3.387714

27	1	0	1.182406	0.599136	3.816312
28	1	0	-1.089445	-1.925425	-1.750093
29	1	0	-1.897898	-2.111797	-0.191618
30	1	0	-2.707224	-0.346177	-2.355584
31	1	0	-1.528789	1.498557	-1.674033
32	1	0	-3.344460	2.794381	-0.743269
33	1	0	-3.676760	1.567870	0.491504
34	1	0	-1.362272	3.566195	0.491065
35	1	0	-2.377465	3.067232	1.848968
36	1	0	2.820564	1.078371	-2.341430
37	1	0	4.739646	0.010140	-0.171923
38	1	0	4.281597	1.736632	-0.480175
39	1	0	3.413471	-0.978394	-3.646654
40	1	0	4.562175	-1.473933	-2.384669
41	1	0	4.844723	0.003356	-3.316936
42	1	0	-0.978057	-3.092835	1.352664
43	1	0	-1.537818	-1.564259	2.015298
44	1	0	-0.255759	-2.463592	2.834864
45	1	0	-6.916725	-0.033211	-1.512806
46	1	0	-6.298934	0.105297	0.166495
47	1	0	-6.400109	-1.494302	-0.605717
48	1	0	1.376954	-3.841245	1.763480
49	1	0	3.391996	-2.107231	-0.171727
50	1	0	2.396639	-2.469707	-1.565139
51	1	0	0.653663	-3.140095	-0.262552
52	1	0	1.623506	-1.407714	2.744827
53	1	0	2.972922	0.789839	2.215922
54	1	0	3.423317	-0.818912	1.639124
55	7	0	2.667655	0.471707	0.191478
56	8	0	0.399880	0.026287	-2.407435
57	8	0	2.031399	-3.324128	1.267432
58	8	0	-4.017149	-1.230362	0.462534
59	8	0	-4.909940	-0.237691	-1.356803
60	1	0	2.190790	1.474840	0.111934
61	17	0	1.966619	3.277937	-0.199344

Conformation BHC-HCl:

Free energy = -1711.047159 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.381162	-1.106771	-0.610879
2	6	0	-1.329424	2.056189	-1.036284
3	6	0	-0.314574	3.165337	-0.916579
4	6	0	0.776388	3.083548	0.174221
5	6	0	-1.579664	-0.965444	0.930513
6	6	0	-2.746333	-1.117360	-0.078217
7	6	0	-2.521820	0.005064	-1.150333
8	6	0	-3.537931	1.136417	-1.399197
9	6	0	-2.627315	2.323804	-1.797724
10	6	0	2.623974	-2.186736	-1.294334
11	6	0	3.008909	-0.887709	-2.052588
12	6	0	1.885305	-1.268942	-0.270639
13	6	0	3.808465	-2.993957	-0.767322
14	6	0	-0.352006	1.469843	2.262000
15	6	0	-4.096873	-1.000000	0.603104
16	6	0	-6.394198	-1.491635	0.384681
17	6	0	2.084238	-1.414716	1.230615
18	6	0	1.299132	-0.366257	2.051361
19	6	0	0.475600	0.682990	1.215186
20	6	0	1.411893	1.695046	0.434266
21	6	0	1.969939	1.219620	-0.923371
22	6	0	-0.448686	-0.107668	0.235678
23	6	0	-1.299172	0.761822	-0.672579
24	1	0	-0.852066	4.114491	-0.785124
25	1	0	0.164106	3.264512	-1.904457
26	1	0	0.381970	3.485910	1.108371

27	1	0	1.583434	3.768772	-0.114825
28	1	0	-1.216098	-1.938388	1.277231
29	1	0	-1.955155	-0.423104	1.799295
30	1	0	-2.711039	-2.086920	-0.577622
31	1	0	-2.296279	-0.493245	-2.101475
32	1	0	-4.288325	0.891262	-2.157126
33	1	0	-4.061645	1.384481	-0.468075
34	1	0	-2.445843	2.337247	-2.884435
35	1	0	-3.060015	3.300071	-1.544550
36	1	0	1.923177	-2.818236	-1.842707
37	1	0	4.058644	-0.740415	-2.315135
38	1	0	2.349114	-0.643380	-2.889048
39	1	0	3.476594	-3.770601	-0.069016
40	1	0	4.545553	-2.358214	-0.265312
41	1	0	4.310186	-3.494724	-1.603199
42	1	0	-0.795195	0.799111	3.004710
43	1	0	-1.167976	2.035654	1.808100
44	1	0	0.283680	2.178844	2.803347
45	1	0	-7.027498	-2.018017	-0.329864
46	1	0	-6.699975	-0.445658	0.472013
47	1	0	-6.452701	-1.961532	1.369913
48	1	0	1.754118	0.730394	3.606118
49	1	0	3.146924	-1.301688	1.466398
50	1	0	1.787841	-2.427109	1.528535
51	1	0	0.552955	-0.903113	2.655361
52	1	0	2.272906	1.854949	1.094110
53	1	0	1.185453	1.146875	-1.683123
54	1	0	2.722430	1.934628	-1.271638
55	7	0	2.648940	-0.082484	-0.830226
56	8	0	-0.131862	-1.781472	-1.483918
57	8	0	2.241085	0.249804	2.919144
58	8	0	-4.321551	-0.431047	1.652301
59	8	0	-5.059273	-1.587293	-0.140872
60	1	0	3.631389	0.087105	-0.287086
61	17	0	5.274560	0.431328	0.237010