

Supplementary Material

Mono-*endo*-6-*N,N*-diethylcarbamoyl and Bis-*endo,endo*-6,12-*N,N*-diethylcarbamoyl derivatives of Tröger's Base. Synthesis and *exo-endo* isomerization study

Sami Dawaigher,^a Emil Lindbäck,^a Daniel Strand,^a Anna Cederbalk,^a Stuart Winikoff,^{*b} Michael Harmata,^{*c} Victor Snieckus,^{*d} and Kenneth Wärnmark^{*a}

^a Centre for Analysis and Synthesis, Department of Chemistry, Lund University.
P. O. Box 124, 22100 Lund, Sweden

^b Department of Chemistry, Truman State University, Kirksville, MO 63501, U.S.A.

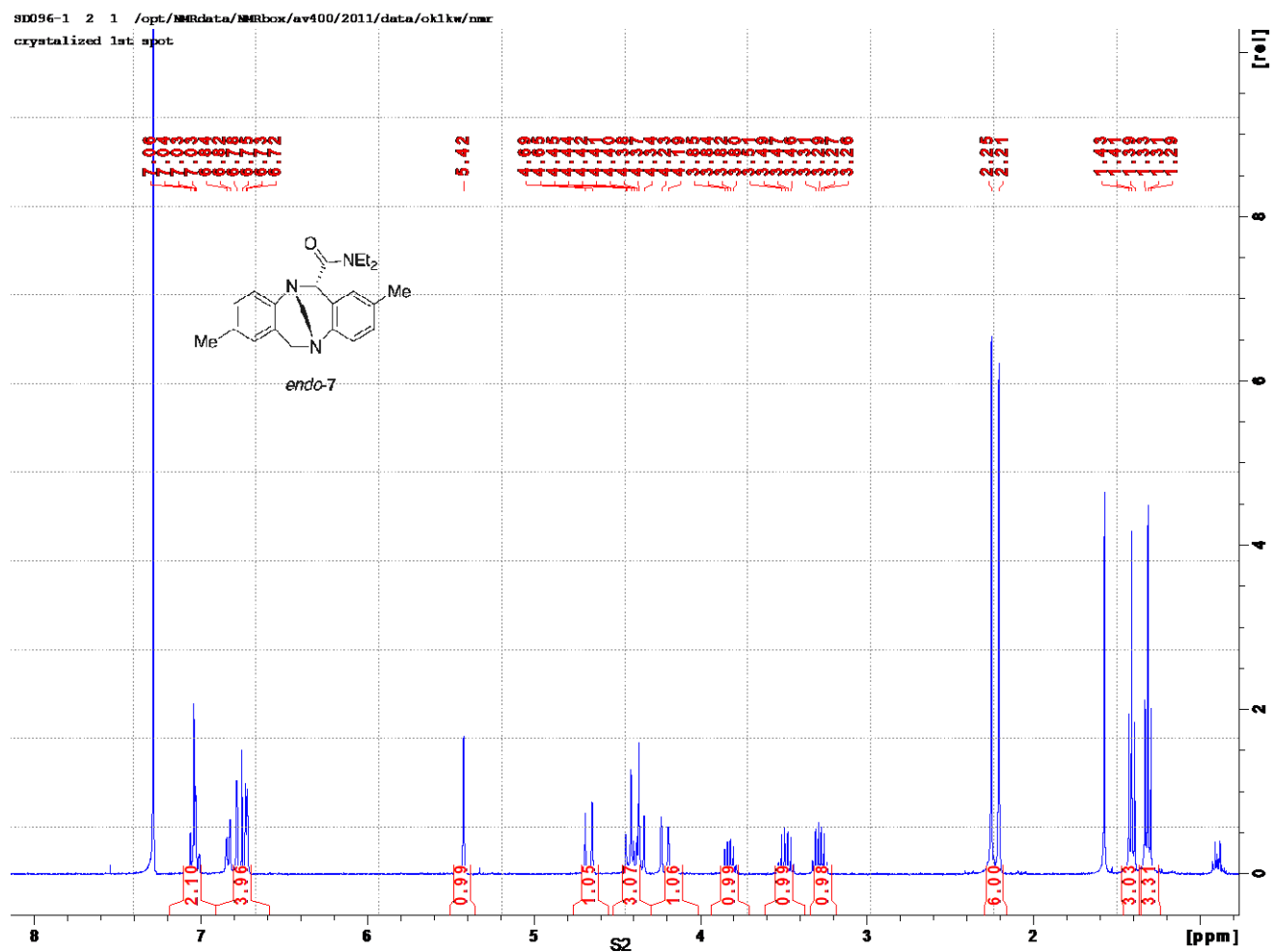
^c Department of Chemistry, University of Missouri, Columbia, MO 65211, U.S.A.

^d Department of Chemistry, Queen's University, Kingston, ON K7L 3N6, Canada

Email: swinikoff@truman.edu; harmatam@missouri.edu; victor.snieckus@chem.queensu.ca; kenneth.warnmark@chem.lu.se

Table of Contents

¹ H and ¹³ C NMR Spectra of <i>endo</i> -7	S2
¹ H and ¹³ C NMR Spectra of <i>endo</i> -8	S4
X-ray Diffraction Data for <i>endo</i> -8	S6
Calculated Pathway Energies	S7
xyz Files for Selected Calculated Structures	S8
References	S26

1. ^1H and ^{13}C NMR Spectra of *endo-7*.Figure S1. ^1H NMR (400 MHz) spectrum of *endo-7* in CDCl_3 .

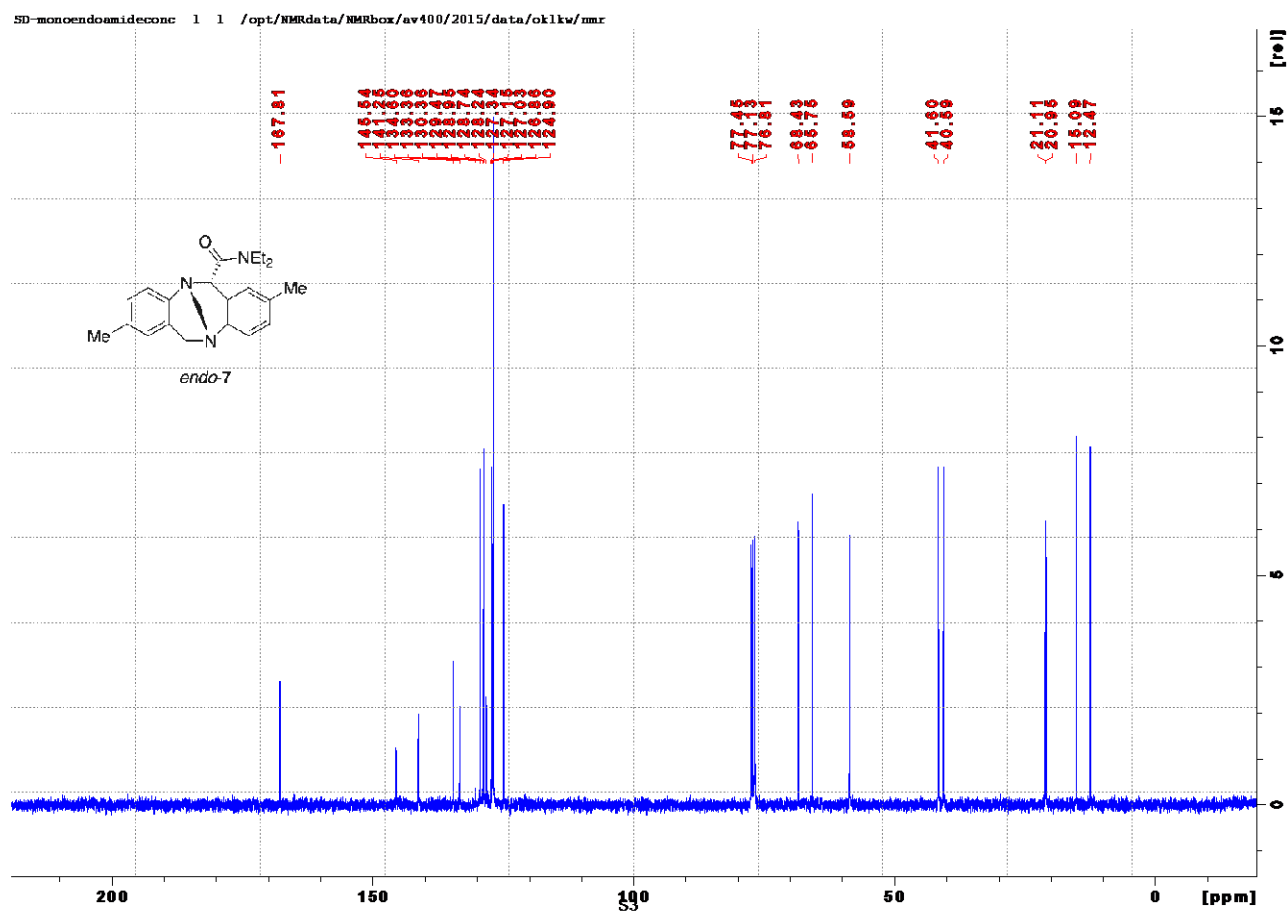


Figure S2. ^{13}C NMR (100 MHz) spectrum of *endo-7* in CDCl_3 .

2. ^1H and ^{13}C NMR Spectra of *endo-8*.

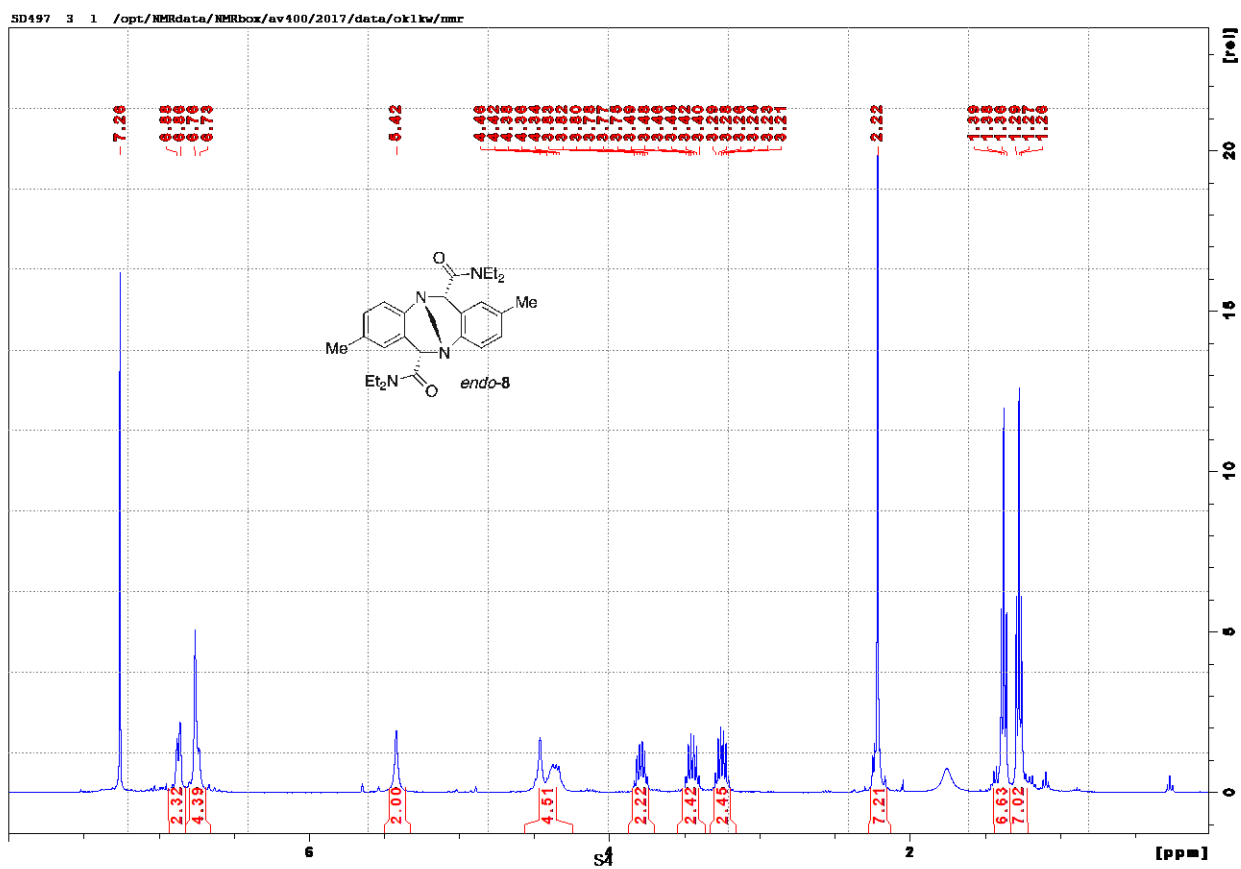


Figure S3. ¹H NMR (400 MHz) spectrum of *endo-8* in CDCl₃.

3. X-ray Diffraction Data for *endo-8*.

A single crystal of *endo-8* grown from EtOAc/heptane was cut to size and mounted on a glass fiber. Data collection was performed at 293 K using an Agilent Xcalibur EOS diffractometer equipped with a Mo $K\alpha$ high-brilliance μ S radiation source ($\lambda = 0.71073 \text{ \AA}$). The structure was solved SUPERFLIP^{S1} and refined with SHELXL-2013.^{S2} Non-hydrogen atoms were refined anisotropically.

Table S1. Crystal data and structure refinement for *endo-8*.

Chemical formula	C ₂₇ H ₃₆ N ₄ O ₂	
Formula mass	448.61	
Crystal size	0.2 x 0.2 x 0.05 mm ³	
Crystal habit	Colorless, plate	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	$a = 11.3586(13) \text{ \AA}$	$\beta = 90^\circ$.
	$b = 9.9446(14) \text{ \AA}$	$\gamma = 102.796(12)^\circ$.
	$c = 22.262(3) \text{ \AA}$	$\alpha = 90^\circ$.
Cell unit volume	2452.1(6) Å ³	
Number of formula units per cell, Z	4	
Density (calculated)	1.215 Mg/m ³	
Absorption coefficient	0.078 mm ⁻¹	
F(000)	968	
Reflections collected	8593	
Independent reflections	2829 [$R_{int} = 0.0568$]	
Data / restraints / parameters	2829/ 0 / 150	
Goodness-of-fit on F^2	0.946	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0735$, $wR2 = 0.1741$	
R indices (all data)	$R_1 = 0.1204$, $wR2 = 0.2061$	
Largest diff. peak and hole	0.224 and -0.195 e.Å ⁻³	
CCDC	1981491	

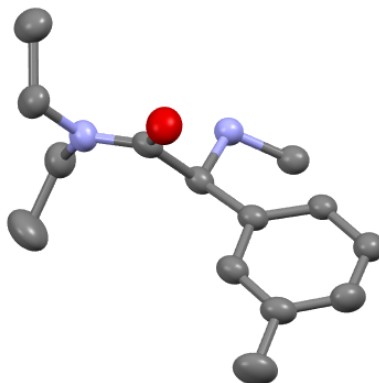


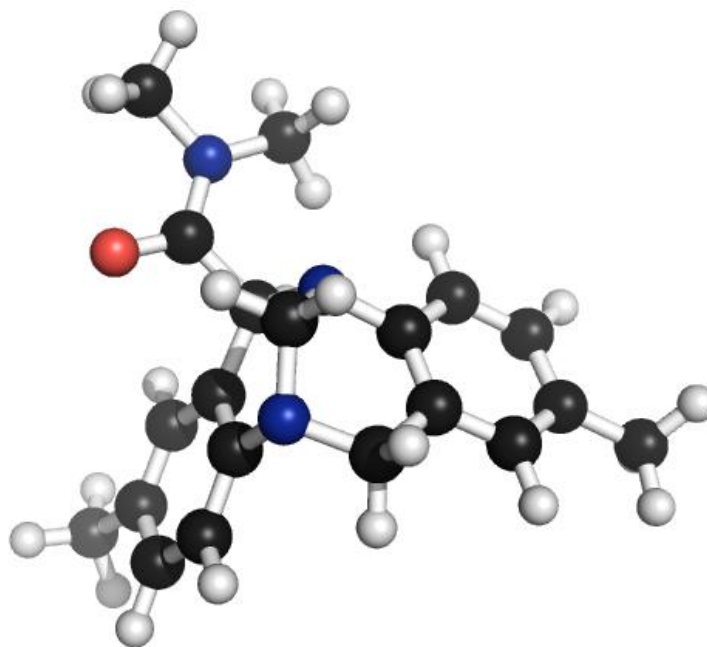
Figure S5. The asymmetric unit of *endo-8*. Gray = carbon atom, blue = nitrogen atom; red = oxygen atom. Thermal ellipsoids are shown at 30% probability. Hydrogen atoms are omitted for clarity.

4. Calculated Pathway Energies

Table S2. Relative Energies of Species shown in Scheme 3 used to calculate the free energy surface in Figure 4.

Entry	Species	Relative Energy (kcal/mol)
1	<i>exo-9</i>	0.0
2	<i>endo-9</i>	2.0
3	<i>exo-10</i>	8.8
4	<i>endo-10</i>	10.3
5	<i>exo-11</i>	19.2
6	<i>endo-11</i>	14.2
7	<i>exo-12</i>	-13.8
8	<i>endo-12</i>	-15.0
9	13	-23.7

5. xyz Files for Selected Calculated Structures

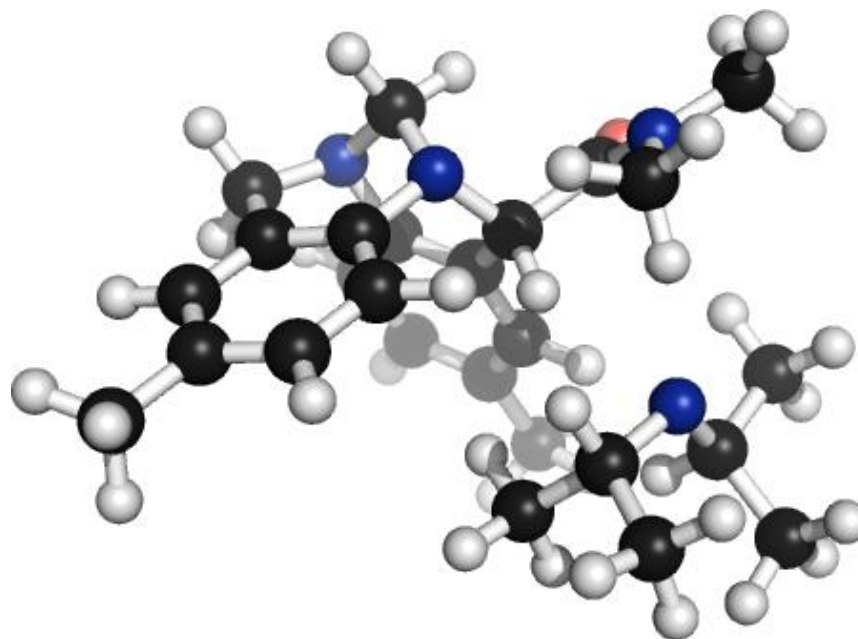
Exo-9

47

Exo-9

H	4.6424681	-0.1471754	0.6037628
C	3.8194090	0.4459524	0.2108416
C	1.7146147	1.8997595	-0.7879503
C	2.5450008	0.2328469	0.7264046
C	4.0678446	1.3586050	-0.8004870
C	2.9832787	2.0824558	-1.2966899
C	1.4762222	0.9794022	0.2292973
H	3.1426467	2.8069988	-2.0896859
H	0.8881197	2.4910676	-1.1673186
C	2.3179607	-0.8117196	1.7841862
H	2.7045535	-0.4694396	2.7506452
H	2.8647305	-1.7240361	1.5337366
N	0.8967811	-1.1191929	1.9363966
N	0.1545393	0.8257251	0.7488123
C	-0.7460587	0.0799873	-0.1445395
H	-0.5546077	0.4150908	-1.1674174
C	-0.4703907	-1.4012046	-0.0869081
C	0.3705192	-1.9288970	0.8906013
C	-1.0164480	-2.2478824	-1.0455172
H	-1.6846703	-1.8245048	-1.7930093
C	0.6918340	-3.2840392	0.8442598

C	-0.7279220	-3.6004176	-1.0849914
H	1.3552481	-3.6889293	1.6017718
C	0.1562547	-4.1018397	-0.1274397
H	0.4125728	-5.1564316	-0.1415872
C	0.1784512	0.1367967	2.0316874
H	0.6704849	0.7667434	2.7748120
H	-0.8480013	-0.0483541	2.3530949
C	-2.1994031	0.4028717	0.2298732
N	-2.6753704	1.6286185	-0.0743529
C	-3.9976173	1.9783282	0.4073203
H	-4.1614687	1.5592868	1.3984513
H	-4.0779079	3.0632607	0.4610790
C	-1.9970671	2.6421150	-0.8497107
H	-2.7275446	3.1504761	-1.4812898
H	-1.2474909	2.2105079	-1.5066710
O	-2.8831598	-0.4164599	0.8259742
C	5.4432765	1.5630575	-1.3502900
H	5.8143098	2.5668114	-1.1267682
H	5.4556264	1.4536431	-2.4372183
H	6.1498425	0.8452725	-0.9313822
C	-1.3476138	-4.5048316	-2.1025391
H	-2.1071453	-5.1463260	-1.6470486
H	-0.6043229	-5.1644664	-2.5559833
H	-1.8321780	-3.9387320	-2.8988055
H	-4.7799597	1.6033053	-0.2590868
H	-1.5131697	3.3857701	-0.2094030

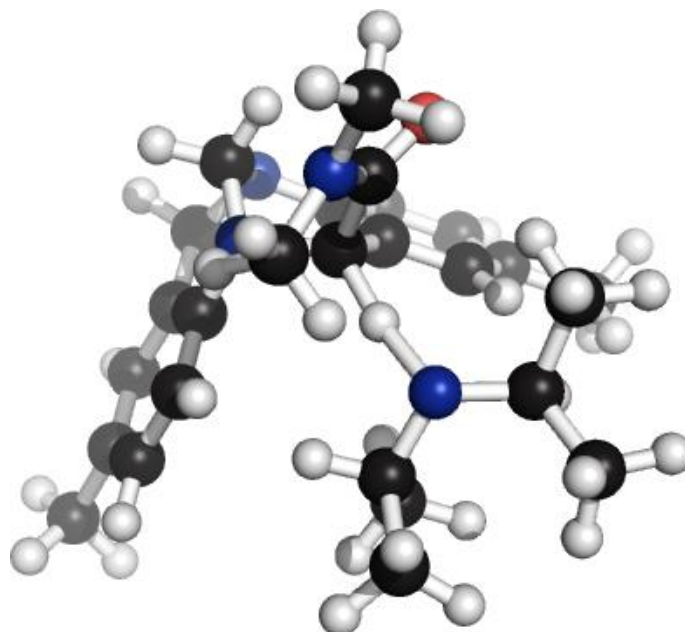
Exo-10

68

Exo-10

C	-1.9854512	-3.8540883	1.2359912
C	-0.5624825	-4.3460727	1.1843483
C	-0.6641736	-1.4258858	-0.7460028
C	0.4990024	-3.4387380	1.2164003
C	0.4804370	-1.2269284	0.2117071
H	-2.4447247	-4.0917848	2.2031301
H	-2.5803941	-4.3624113	0.4732716
H	1.4169804	-1.5055215	-0.2967217
C	-1.8540448	-2.0235455	-0.3296585
C	-0.5195168	-1.0590852	-2.0780086
H	0.4218121	-0.6125385	-2.3870366
C	-1.5126821	-1.2750358	-3.0170133
C	-2.6917740	-1.8853819	-2.5869431
C	-2.8599110	-2.2522594	-1.2669131
H	-3.7857915	-2.7131528	-0.9348904
C	1.7974634	-3.9165011	1.0593210
H	2.6197561	-3.2113596	1.0562771
C	2.0410254	-5.2653030	0.9114870
C	0.9987517	-6.1918745	0.9276702
C	-0.2913114	-5.7042642	1.0626453
H	-1.1278910	-6.4010895	1.0513063
N	-2.0614130	-2.4092571	1.0281418
N	0.2765111	-2.0462799	1.4197570
C	-1.0733456	-1.7976504	1.8997747
H	-1.1935157	-2.2126353	2.9034296

H	-1.2361247	-0.7199334	1.9501951
C	0.6410316	0.2523130	0.5882869
N	1.7516003	0.5940578	1.2734948
O	-0.2169116	1.0752322	0.2899418
C	1.9575240	1.9962045	1.5588867
H	2.6054176	2.0909809	2.4297877
H	2.4241466	2.5111411	0.7114039
H	1.0049051	2.4791332	1.7672228
C	2.9044727	-0.2840493	1.4085846
H	3.3353052	-0.4810277	0.4121222
H	3.6368991	0.2154521	2.0417912
H	2.6170204	-1.2152374	1.8978380
N	3.3377732	-0.8119615	-1.7142573
C	3.6895833	-2.1977942	-1.7541114
H	3.6708879	-2.5410725	-0.6986463
C	2.9919849	-0.1722105	-2.9340971
H	2.1575500	-0.6840534	-3.4850637
C	4.1089130	-0.0306606	-3.9882685
H	3.7938900	0.5986995	-4.8303621
H	4.9924670	0.4241010	-3.5237646
H	4.4096606	-0.9991450	-4.3906089
C	2.4866283	1.2281217	-2.6138217
H	3.2887986	1.7906376	-2.1216937
H	2.1788857	1.7742541	-3.5128784
H	1.6402792	1.1976709	-1.9214410
C	5.1177801	-2.5487300	-2.2203901
H	5.8279413	-1.8443223	-1.7792872
H	5.3976751	-3.5650553	-1.9139922
H	5.2257921	-2.4934451	-3.3071283
C	2.7056933	-3.1133549	-2.4920180
H	2.6809700	-2.8840492	-3.5635965
H	2.9823894	-4.1682133	-2.3870865
H	1.6886219	-2.9913208	-2.1034211
C	-1.3278493	-0.8667814	-4.4446333
H	-1.6337798	-1.6594055	-5.1312007
H	-1.9278222	0.0146933	-4.6891029
H	-0.2818603	-0.6243699	-4.6490416
C	1.2693030	-7.6538357	0.7666829
H	1.3721291	-7.9254857	-0.2882070
H	2.2010846	-7.9419736	1.2590244
H	0.4622697	-8.2587480	1.1830219
H	3.0626102	-5.6142943	0.7912676
H	-3.4900514	-2.0653226	-3.3015415

Exo-11

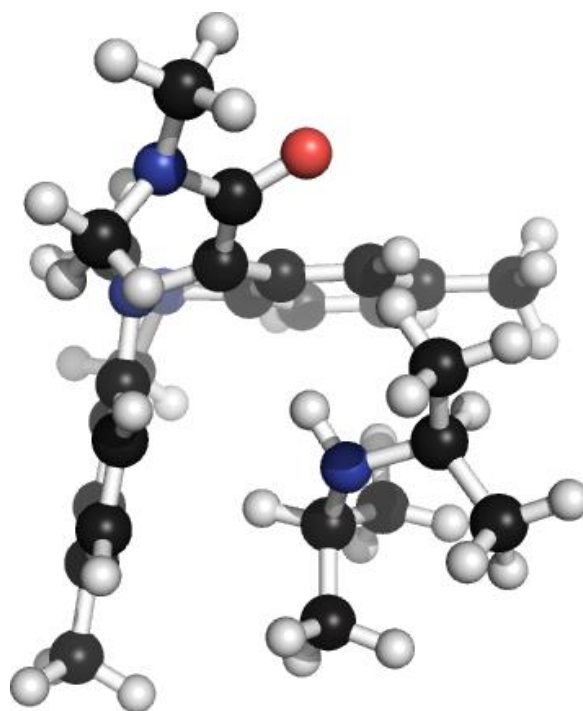
68

Exo-11

C	-1.8726655	-3.7749819	1.1931288
C	-0.4618935	-4.2955865	1.1112265
C	-0.5576750	-1.3753429	-0.8532736
C	0.6228457	-3.4090352	1.0992647
C	0.6289964	-1.1656709	0.0391162
H	-2.3102232	-3.9958153	2.1754099
H	-2.5029448	-4.2768822	0.4542978
H	1.7646782	-1.1872028	-0.7496419
C	-1.7401893	-1.9763501	-0.3972434
C	-0.5008043	-1.0244651	-2.1997171
H	0.4086326	-0.5674703	-2.5629022
C	-1.5237585	-1.2622134	-3.0987432
C	-2.6790049	-1.8821565	-2.6236866
C	-2.7810476	-2.2259740	-1.2903515
H	-3.6919884	-2.6817735	-0.9108385
C	1.9053004	-3.9393241	0.9930539
H	2.7441161	-3.2566967	1.0144461
C	2.1138966	-5.2978017	0.8886012
C	1.0455229	-6.1938787	0.9115675
C	-0.2290646	-5.6643413	1.0339160
H	-1.0860962	-6.3364549	1.0520139
N	-1.9177773	-2.3337032	0.9726249
N	0.4454591	-2.0096446	1.2544829
C	-0.8794005	-1.7394768	1.7977611
H	-0.9711661	-2.1550650	2.8065133

H	-1.0293013	-0.6605160	1.8598892
C	0.7528263	0.2671884	0.4683320
N	1.7890694	0.5987168	1.2904797
O	-0.0226681	1.1424709	0.0800377
C	1.9644389	2.0025954	1.5853131
H	2.5972565	2.1060306	2.4661923
H	2.4298996	2.5395815	0.7499602
H	1.0012291	2.4704500	1.7823387
C	2.9299708	-0.2712046	1.5172940
H	3.4172064	-0.5112196	0.5633942
H	3.6343489	0.2481200	2.1660539
H	2.6212996	-1.1957722	2.0051136
N	2.9832507	-0.9677487	-1.6160649
C	3.5057659	-2.3115219	-1.7131643
H	3.4645015	-2.6894096	-0.6814387
C	2.8005484	-0.2317708	-2.8435600
H	2.0107927	-0.6733579	-3.4974188
C	4.0092741	-0.0974684	-3.7789281
H	3.7726946	0.6047133	-4.5859465
H	4.8819378	0.2897250	-3.2405117
H	4.2920819	-1.0408029	-4.2458705
C	2.3545306	1.1819748	-2.5035727
H	3.1816369	1.7112251	-2.0159544
H	2.0773489	1.7377639	-3.4061205
H	1.5040325	1.2015907	-1.8195996
C	4.9795965	-2.4902247	-2.1081185
H	5.6061676	-1.7274404	-1.6383316
H	5.3365282	-3.4731976	-1.7828386
H	5.1401878	-2.4373816	-3.1867768
C	2.6404515	-3.2577159	-2.5419790
H	2.6503222	-2.9743068	-3.5999173
H	2.9879183	-4.2939649	-2.4690218
H	1.6039230	-3.2154714	-2.1925041
C	-1.3790619	-0.8606555	-4.5334620
H	-1.7118602	-1.6505000	-5.2106785
H	-1.9713442	0.0297630	-4.7646049
H	-0.3357822	-0.6314374	-4.7662268
C	1.2748074	-7.6653408	0.7785835
H	1.3550950	-7.9607031	-0.2718825
H	2.2064720	-7.9671324	1.2631626
H	0.4588151	-8.2415118	1.2181115
H	3.1272668	-5.6795682	0.8023239
H	-3.5038781	-2.0832693	-3.3014839

Exo-12



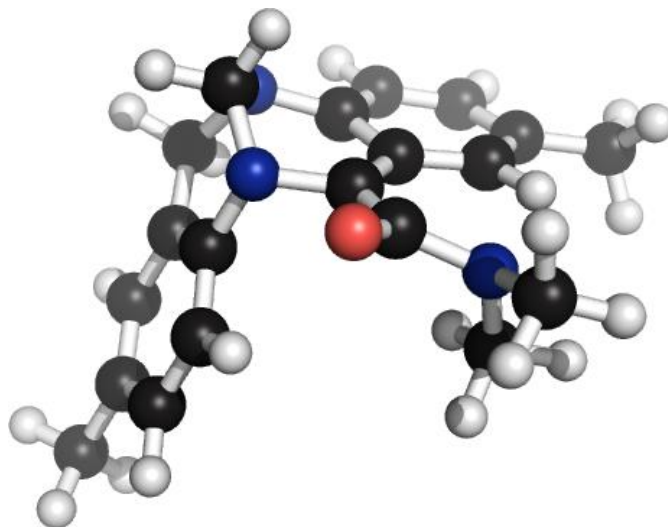
68

Exo-12

C	-1.3899075	-4.0296244	0.7420847
C	0.0979348	-4.0740604	0.9738458
C	-0.5729131	-1.0087822	-0.7083486
C	0.7954556	-2.8936836	1.2520334
C	0.2328197	-0.6777377	0.4537675
H	-1.9277280	-4.5293145	1.5576909
H	-1.6327753	-4.5741213	-0.1748129
H	2.1213981	-1.5552179	-1.2313017
C	-1.5566153	-2.0306065	-0.6209531
C	-0.4422070	-0.3815286	-1.9643996
H	0.2916318	0.4089319	-2.0634566
C	-1.1697960	-0.7485329	-3.0796531
C	-2.1029711	-1.7804209	-2.9651950
C	-2.2895162	-2.3973370	-1.7421121
H	-3.0446164	-3.1714637	-1.6281757
C	2.1911517	-2.9447750	1.2761444
H	2.7475692	-2.0255079	1.4029470
C	2.8624791	-4.1385716	1.1206273
C	2.1765364	-5.3358610	0.9157786
C	0.7947233	-5.2704455	0.8326701
H	0.2304117	-6.1773787	0.6184162
N	-1.8768964	-2.6582774	0.6296286
N	0.1106092	-1.6759147	1.4998249

C	-1.3000809	-1.9202132	1.7391429
H	-1.4500300	-2.5079940	2.6515923
H	-1.7912937	-0.9522832	1.8587308
C	0.5606754	0.6673420	0.7587830
N	1.0761708	1.0174941	2.0385061
O	0.3684807	1.6093637	-0.0370727
C	1.3283693	2.4326058	2.2025386
H	1.5275136	2.6324979	3.2584462
H	2.1928752	2.7829746	1.6181227
H	0.4669301	3.0191305	1.8907423
C	2.1153514	0.2161632	2.6453048
H	3.0172674	0.1651382	2.0129186
H	2.4076852	0.6696131	3.5950040
H	1.7699335	-0.7943693	2.8416653
N	2.7678479	-1.9332661	-1.9228294
C	2.3582927	-3.3102676	-2.2233073
H	1.9100236	-3.6638379	-1.2899283
C	2.9027001	-0.9558553	-2.9920816
H	1.9699179	-0.8710835	-3.5818756
C	4.0295543	-1.3040773	-3.9460783
H	4.1923368	-0.4848316	-4.6506770
H	4.9568260	-1.4668409	-3.3875158
H	3.8226918	-2.2020698	-4.5305142
C	3.1660760	0.3967253	-2.3525539
H	4.1009924	0.3650334	-1.7844619
H	3.2608773	1.1738155	-3.1161846
H	2.3653688	0.6831405	-1.6644710
C	3.5460766	-4.2189033	-2.4949483
H	4.3020236	-4.0995738	-1.7145019
H	3.2238259	-5.2645308	-2.5057421
H	4.0190383	-4.0116535	-3.4581779
C	1.2954648	-3.4556197	-3.3018204
H	1.6625261	-3.1533741	-4.2878472
H	0.9860235	-4.5023742	-3.3756832
H	0.4127117	-2.8561096	-3.0681285
C	-0.9404566	-0.0857504	-4.4031016
H	-0.6473246	-0.8171321	-5.1627819
H	-1.8448818	0.4058790	-4.7740874
H	-0.1524277	0.6678989	-4.3384937
C	2.9207636	-6.6190204	0.7227653
H	3.3469828	-6.6812158	-0.2837092
H	3.7551178	-6.7051379	1.4232388
H	2.2702023	-7.4836285	0.8617791

H 3.9486523 -4.1482641 1.1515919
H -2.6841013 -2.0869760 -3.8300044

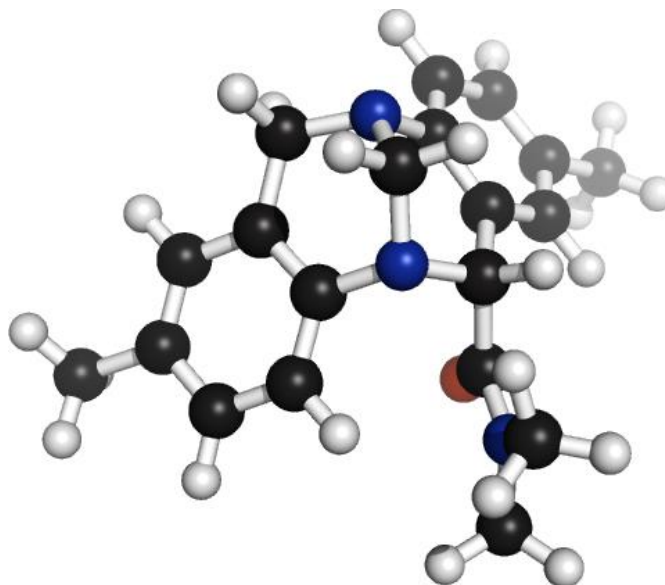


46

13

H -1.2931327 -3.9977444 0.7103050
C -1.5926317 -2.9514291 0.7192918
C -2.2905664 -0.2899618 0.7538784
C -1.0071456 -2.0839129 -0.1990515
C -2.5134969 -2.5204336 1.6592040
C -2.8483148 -1.1642935 1.6628990
C -1.3736173 -0.7381341 -0.1969779
H -3.5645341 -0.7976812 2.3934367
H -2.5522244 0.7630023 0.7501556
C 0.0327850 -2.5764632 -1.1717369
H -0.4424502 -3.1898515 -1.9485018
H 0.7507260 -3.2224444 -0.6592861
N 0.7484109 -1.4821004 -1.8217401
N -0.8161147 0.1811964 -1.1256785
C 1.4761186 0.4195624 -0.3759248
C 1.7272669 -0.8452583 -0.9851951
C 2.5683070 0.9887029 0.3227731
H 2.4111239 1.9536316 0.7872284
C 2.9547690 -1.4720613 -0.8336928
C 3.7915919 0.3610352 0.4646056
H 3.0971408 -2.4317784 -1.3252331
C 3.9843635 -0.8971252 -0.1092285
H 4.9375843 -1.4068060 -0.0023168
C -0.2452172 -0.5177539 -2.2575535

H	-1.0238830	-1.0548456	-2.8089085
H	0.2102525	0.2203921	-2.9219973
C	-3.1154705	-3.4618198	2.6549579
H	-4.2061745	-3.4764198	2.5847775
H	-2.8663589	-3.1706085	3.6789112
H	-2.7578598	-4.4815585	2.5034125
C	4.9017760	1.0119791	1.2317896
H	4.6158307	2.0065932	1.5769930
H	5.8028794	1.1118163	0.6201061
H	5.1845082	0.4202597	2.1073072
C	0.1852385	1.0389938	-0.5200292
C	-0.1526677	2.3383830	-0.0867037
N	-1.3924089	2.8985633	-0.5204121
C	-1.7339063	4.1510097	0.1101354
H	-1.0947085	4.9864143	-0.2165335
H	-1.6414401	4.0762220	1.1922078
C	-1.6087655	2.9527407	-1.9493277
H	-2.6323497	3.2772254	-2.1579627
H	-1.4669660	1.9720173	-2.3963217
O	0.5467037	3.0318231	0.6821079
H	-0.9257127	3.6701600	-2.4360453
H	-2.7692593	4.3987615	-0.1401246

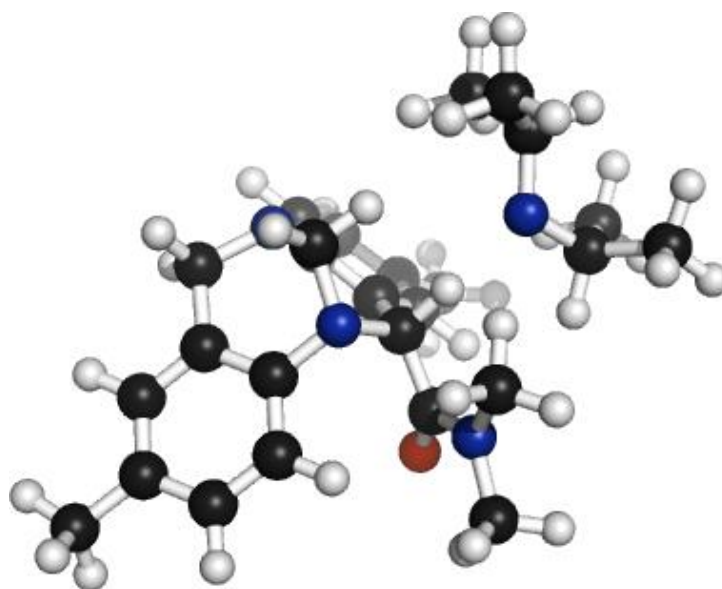
Endo-9

47

Endo-9

C	-1.65284840	-2.99705520	1.86930200
C	-0.47148170	-3.91771450	2.01334040
C	0.03754500	-1.86235370	-0.86052730
C	0.82582830	-3.46822750	1.75004430
C	1.31683270	-1.85111680	-0.05814660
H	-2.06258880	-2.75683970	2.85733010
H	-2.45230820	-3.49050440	1.31276010
H	1.74400790	-0.84212830	-0.11659850
C	-1.19926790	-1.86357380	-0.21662130
C	0.05093020	-1.83453850	-2.25358960
H	1.00213390	-1.79312710	-2.77509290
C	-1.11691610	-1.88574070	-2.98413790
C	-2.35610750	-1.96379980	-2.34496180
C	-2.37491720	-1.93665300	-0.96210130
H	-3.32269910	-1.93991770	-0.42934950
C	1.89538180	-4.34150940	1.91777280
H	2.90338930	-3.97325230	1.74907240
C	1.71361580	-5.65789720	2.31275510
C	0.41823080	-6.09227760	2.57731430
C	-0.65086440	-5.22771200	2.43617690
H	-1.65894530	-5.57408650	2.64776650
N	-1.29273160	-1.75078420	1.19772780
N	1.06901570	-2.10839640	1.37468850
C	-0.05116950	-1.26803170	1.76590180
H	-0.14204580	-1.26068390	2.85397860

H	0.14328270	-0.24831290	1.42595020
C	2.36012100	-2.83034410	-0.60524220
N	3.65078640	-2.60460310	-0.26278950
O	2.02710450	-3.77192840	-1.30254410
C	4.13206240	-1.56445120	0.62050690
H	4.79620210	-2.01168520	1.36643350
H	4.70596750	-0.81604760	0.06643840
H	3.32032450	-1.08172420	1.15562860
C	4.65994950	-3.55883350	-0.66715990
H	5.55026250	-3.02831730	-1.01244220
H	4.94541070	-4.19698520	0.17787660
H	4.27887420	-4.18711870	-1.46715140
H	2.55443384	-6.31322230	2.40480966
H	-3.25761006	-2.03512426	-2.91689357
C	0.18049146	-7.54257138	3.03745335
H	-0.55455149	-7.55413300	3.81493531
H	-0.16568408	-8.12688209	2.21062598
H	1.09652752	-7.95437029	3.40650564
C	-1.05930957	-1.86665931	-4.52294178
H	-0.86066259	-2.85386615	-4.88469035
H	-1.99678424	-1.52660749	-4.91076390
H	-0.28045654	-1.20624641	-4.84253958

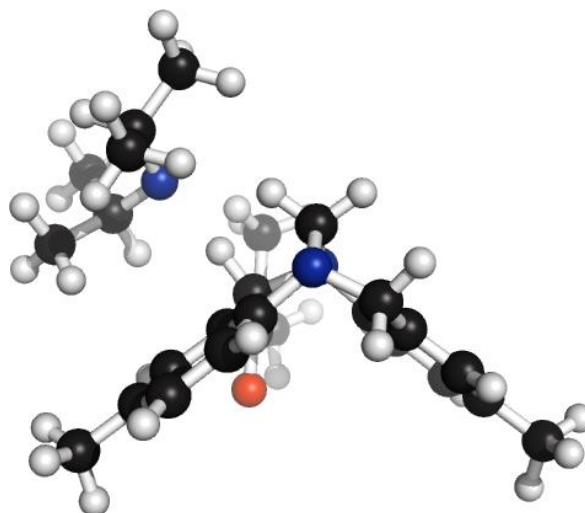
Endo-10

68

Endo-10

H	-1.4588721	-4.1387060	0.4942962
C	-1.7393635	-3.0876004	0.4715164
C	-2.4136670	-0.4245629	0.3971485
C	-1.0095410	-2.2248517	-0.3386336
C	-2.7935717	-2.6513073	1.2558322
C	-3.1141477	-1.2942246	1.2068096
C	-1.3511477	-0.8715954	-0.3909643
H	-3.9419435	-0.9225806	1.8037785
H	-2.6992233	0.6207477	0.3459478
C	0.1328353	-2.7566435	-1.1617808
H	-0.2539240	-3.3941996	-1.9659922
H	0.7763351	-3.3906803	-0.5456233
N	0.9296032	-1.6867683	-1.7521017
N	-0.6809911	0.0208873	-1.2750902
C	1.5585341	0.1777791	-0.2623673
C	1.8249609	-1.0759740	-0.8227610
C	2.5316673	0.7615079	0.5407998
H	2.3531500	1.7555317	0.9397250
C	3.0017019	-1.7388437	-0.4942362
C	3.7168519	0.1171436	0.8625907
H	3.1880336	-2.7125333	-0.9372440
C	3.9312557	-1.1579473	0.3464639
H	4.8507180	-1.6849646	0.5842023
C	0.0131764	-0.7090447	-2.3181019
H	-0.7048877	-1.2384923	-2.9500029
H	0.5628599	0.0177505	-2.9211941

C	-3.5704207	-3.5906708	2.1217087
H	-4.6279491	-3.6003870	1.8452664
H	-3.5213307	-3.2977443	3.1735475
H	-3.1923387	-4.6108792	2.0405314
C	4.7208091	0.7808170	1.7529359
H	4.7862519	1.8507821	1.5415329
H	5.7152539	0.3477126	1.6305446
H	4.4503908	0.6794381	2.8082037
C	0.3242796	0.9263761	-0.6738992
H	0.6791462	1.5790867	-1.5183337
C	-0.3174082	1.7722585	0.4050690
N	-1.2176457	2.6917315	-0.0245444
C	-2.0657480	3.3579234	0.9352789
H	-1.8603709	4.4322179	0.9643565
H	-1.9033029	2.9380261	1.9248037
C	-1.5184318	2.9819676	-1.4112042
H	-2.3971847	2.4170871	-1.7459455
H	-0.6747007	2.7744732	-2.0790996
O	-0.0785373	1.6110612	1.5957517
H	-1.7497395	4.0476223	-1.4907573
H	-3.1162293	3.2221963	0.6548333
N	1.4410849	2.6311639	-2.9134665
C	1.8864681	3.7426725	-2.1335395
H	1.2820454	3.7443081	-1.2026951
C	2.2263390	2.3420974	-4.0697198
H	2.8659933	3.2008827	-4.3767514
C	3.1825786	1.1505290	-3.8915110
H	2.6013531	0.2437754	-3.6808954
H	3.7964932	0.9614527	-4.7824257
H	3.8484508	1.3040268	-3.0385181
C	1.3186061	2.0550493	-5.2622159
H	0.6512984	1.2227555	-5.0125953
H	0.6897728	2.9254142	-5.4666225
H	1.8734669	1.7892300	-6.1714459
C	1.6124864	5.1025972	-2.8009131
H	0.5555540	5.1616538	-3.0728718
H	1.8595049	5.9555215	-2.1557707
H	2.1977176	5.2004571	-3.7224995
C	3.3469524	3.7079765	-1.6593452
H	3.5939687	4.5682850	-1.0255770
H	3.5407446	2.7931777	-1.0898126
H	4.0309261	3.7225022	-2.5151257

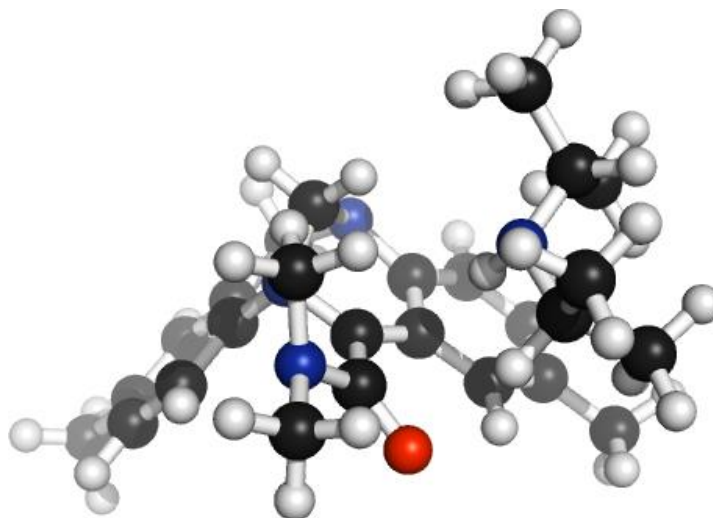
Endo 11

68

Endo-11

H	-1.51198660	-4.36287090	0.66789680
C	-1.81739470	-3.31814880	0.67287200
C	-2.52464850	-0.65971370	0.70586340
C	-1.23462710	-2.44935610	-0.24675960
C	-2.73831360	-2.88899470	1.61410620
C	-3.07968360	-1.53430330	1.61577630
C	-1.60573920	-1.10528860	-0.24399430
H	-3.79441270	-1.16806960	2.34796840
H	-2.78548050	0.39336300	0.70536450
C	-0.18984560	-2.93424790	-1.21862400
H	-0.66195370	-3.53854760	-2.00462430
H	0.52480820	-3.58655860	-0.70925010
N	0.53287250	-1.83628070	-1.85530610
N	-1.03789150	-0.17831860	-1.15849490
C	1.24728300	0.05029540	-0.38260600
C	1.50917290	-1.20382680	-1.01099150
C	2.34627760	0.63353490	0.29710750
H	2.18898930	1.60169840	0.75647490
C	2.74746380	-1.81344670	-0.88618120
C	3.57946140	0.02194430	0.41082150
H	2.89611520	-2.76373620	-1.39433600
C	3.78043650	-1.23012980	-0.17406930
H	4.74285610	-1.72650310	-0.08701910
C	-0.45102000	-0.86340780	-2.29047960
H	-1.22239730	-1.38719250	-2.86436840
H	0.02234660	-0.11453990	-2.93293740

C	-3.33155070	-3.82904920	2.61666480
H	-4.42269460	-3.84701880	2.55362730
H	-3.07704960	-3.53348640	3.63813230
H	-2.97105690	-4.84796920	2.46684840
C	4.70084330	0.68606380	1.14889040
H	4.41929670	1.68274390	1.49306770
H	5.58706960	0.78470610	0.51520690
H	5.00583170	0.10390480	2.02363640
C	-0.04513300	0.66187220	-0.51649270
H	1.14170978	1.44929486	-1.38842720
C	-0.38831630	1.96032410	-0.07023610
N	-1.56075240	2.57330320	-0.58201900
C	-1.92250860	3.82167760	0.04015800
H	-1.27730830	4.65988170	-0.27126300
H	-1.85599950	3.74520260	1.12382850
C	-1.76361740	2.60490740	-2.01489220
H	-2.78945150	2.91790340	-2.23192910
H	-1.61156130	1.62002230	-2.44741550
O	0.27072010	2.60398030	0.77273360
H	-1.07238810	3.30933970	-2.50886270
H	-2.95136280	4.06910340	-0.23614600
N	1.69187800	2.84957740	-2.54510390
C	1.96919020	4.05567100	-1.78102500
H	1.26344390	4.01852350	-0.94196660
C	2.59430210	2.46575020	-3.62061270
H	3.20557630	3.34047490	-3.87639850
C	3.52099380	1.32749630	-3.22417330
H	2.92998450	0.44875770	-2.93563830
H	4.17588540	1.03671680	-4.05063940
H	4.14170370	1.59054010	-2.36485430
C	1.78060100	2.09044170	-4.84862340
H	1.14753450	1.22692260	-4.61861530
H	1.12013780	2.91404400	-5.12939130
H	2.41667740	1.83369560	-5.70089990
C	1.65268430	5.29109580	-2.60651800
H	0.64339930	5.21683090	-3.01795170
H	1.72650360	6.19987570	-2.00441130
H	2.34644160	5.40018790	-3.44756100
C	3.37056280	4.13505950	-1.18909470
H	3.48026940	5.02768460	-0.56834620
H	3.57870860	3.25847970	-0.56993740
H	4.13513280	4.18817850	-1.97300350

Endo-12

68

Endo-12

H	-1.5119866	-4.3628709	0.6678968
C	-1.8173947	-3.3181488	0.6728720
C	-2.5246485	-0.6597137	0.7058634
C	-1.2346271	-2.4493561	-0.2467596
C	-2.7383136	-2.8889947	1.6141062
C	-3.0796836	-1.5343033	1.6157763
C	-1.6057392	-1.1052886	-0.2439943
H	-3.7944127	-1.1680696	2.3479684
H	-2.7854805	0.3933630	0.7053645
C	-0.1898456	-2.9342479	-1.2186240
H	-0.6619537	-3.5385476	-2.0046243
H	0.5248082	-3.5865586	-0.7092501
N	0.5328725	-1.8362807	-1.8553061
N	-1.0378915	-0.1783186	-1.1584949
C	1.2472830	0.0502954	-0.3826060
C	1.5091729	-1.2038268	-1.0109915
C	2.3462776	0.6335349	0.2971075
H	2.1889893	1.6016984	0.7564749
C	2.7474638	-1.8134467	-0.8861812
C	3.5794614	0.0219443	0.4108215
H	2.8961152	-2.7637362	-1.3943360
C	3.7804365	-1.2301298	-0.1740693
H	4.7428561	-1.7265031	-0.0870191
C	-0.4510200	-0.8634078	-2.2904796
H	-1.2223973	-1.3871925	-2.8643684
H	0.0223466	-0.1145399	-2.9329374

C	-3.3315507	-3.8290492	2.6166648
H	-4.4226946	-3.8470188	2.5536273
H	-3.0770496	-3.5334864	3.6381323
H	-2.9710569	-4.8479692	2.4668484
C	4.7008433	0.6860638	1.1488904
H	4.4192967	1.6827439	1.4930677
H	5.5870696	0.7847061	0.5152069
H	5.0058317	0.1039048	2.0236364
C	-0.0451330	0.6618722	-0.5164927
H	1.5014164	2.0659398	-1.9274374
C	-0.3883163	1.9603241	-0.0702361
N	-1.5607524	2.5733032	-0.5820190
C	-1.9225086	3.8216776	0.0401580
H	-1.2773083	4.6598817	-0.2712630
H	-1.8559995	3.7452026	1.1238285
C	-1.7636174	2.6049074	-2.0148922
H	-2.7894515	2.9179034	-2.2319291
H	-1.6115613	1.6200223	-2.4474155
O	0.2707201	2.6039803	0.7727336
H	-1.0723881	3.3093397	-2.5088627
H	-2.9513628	4.0691034	-0.2361460
N	1.6918780	2.8495774	-2.5451039
C	1.9691902	4.0556710	-1.7810250
H	1.2634439	4.0185235	-0.9419666
C	2.5943021	2.4657502	-3.6206127
H	3.2055763	3.3404749	-3.8763985
C	3.5209938	1.3274963	-3.2241733
H	2.9299845	0.4487577	-2.9356383
H	4.1758854	1.0367168	-4.0506394
H	4.1417037	1.5905401	-2.3648543
C	1.7806010	2.0904417	-4.8486234
H	1.1475345	1.2269226	-4.6186153
H	1.1201378	2.9140440	-5.1293913
H	2.4166774	1.8336956	-5.7008999
C	1.6526843	5.2910958	-2.6065180
H	0.6433993	5.2168309	-3.0179517
H	1.7265036	6.1998757	-2.0044113
H	2.3464416	5.4001879	-3.4475610
C	3.3705628	4.1350595	-1.1890947
H	3.4802694	5.0276846	-0.5683462
H	3.5787086	3.2584797	-0.5699374
H	4.1351328	4.1881785	-1.9730035

6. References.

- S1. Palatinus, L.; Chapuis, G. J. *Appl. Cryst.* **2007**, *40*, 786–790.
- S2. Sheldrick, G. M. *Acta Cryst A.* **2008**, *64*, 112–122.