JO001720R

RECEIVED
AUG 28 2001
Journal of Organic Chemistry

Conformation and Configuration of Tertiary Amines via GIAO Derived ^{13}C NMR Chemical Shifts and a Multiple Independent Variable Regression Analysis

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Supporting Information

MM3 Steric Energies and Final Geometries for All Structures

N-methyl piperidine, **1**

FINAL STERIC ENERGY IS 11.9225 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	.32023	1.20684	.19603	(1)
C(2)	-1.15347	1.25779	-.21694	(1)
C(3)	-1.89534	.00000	.24632	(1)
C(4)	-1.15347	-1.25779	-.21694	(1)
C(5)	.32023	-1.20684	.19603	(1)
N(6)	.97898	.00000	-.30494	(8)
C(7)	2.40179	.00000	.02300	(1)
H(8)	.40093	1.25546	1.31822	(5)
H(9)	.83776	2.10761	-.20449	(5)
H(10)	-1.63934	2.16562	.20844	(5)
H(11)	-1.22492	1.34385	-1.32569	(5)
H(12)	-2.93791	.00000	-.14707	(5)
H(13)	-1.96935	.00000	1.35845	(5)
H(14)	-1.63934	-2.16562	.20844	(5)
H(15)	-1.22492	-1.34385	-1.32569	(5)
H(16)	.83776	-2.10761	-.20449	(5)
H(17)	.40093	-1.25546	1.31822	(5)
H(18)	2.90092	.89557	-.40585	(5)
H(19)	2.90091	-.89557	-.40585	(5)
H(20)	2.56666	.00000	1.13529	(5)

2-methyl-1-azabicyclo[2.2.2]octane, **2**

FINAL STERIC ENERGY IS 29.1878 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	.92331	-.63597	-1.37596	(1)
C(2)	.04281	.63213	-1.42588	(1)
N(3)	-.34640	1.05607	-.07779	(8)

C(4)	.86522	1.32952	.69997	(1)
C(5)	1.69670	.04039	.88934	(1)
C(6)	1.04074	-1.09176	.08515	(1)
C(7)	-.38281	-1.30361	.62234	(1)
C(8)	-1.15050	.04232	.62147	(1)
C(9)	-2.54784	-.08452	.00403	(1)
H(10)	1.93338	-.42528	-1.79479	(5)
H(11)	.47674	-1.44284	-2.00003	(5)
H(12)	.59459	1.45659	-1.93005	(5)
H(13)	-.86014	.45311	-2.04745	(5)
H(14)	1.47301	2.10711	.18589	(5)
H(15)	.59126	1.75927	1.68898	(5)
H(16)	1.74432	-.23558	1.96719	(5)
H(17)	2.74492	.20163	.55009	(5)
H(18)	1.63745	-2.03075	.16026	(5)
H(19)	-.34757	-1.72133	1.65405	(5)
H(20)	-.91068	-2.05656	-.00471	(5)
H(21)	-1.28710	.37848	1.67741	(5)
H(22)	-3.19180	-.76177	.60806	(5)
H(23)	-2.52756	-.49739	-1.02732	(5)
H(24)	-3.06376	.90032	-.04114	(5)

1,5-diazabicyclo[3.3.1]nonane, **3**

FINAL STERIC ENERGY IS 23.9394 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
N(1)	.00000	-1.19760	-.61104	(8)
C(2)	-1.23770	-1.27135	.16457	(1)
C(3)	-1.54832	.00000	.96334	(1)
C(4)	-1.23770	1.27135	.16457	(1)
N(5)	.00000	1.19760	-.61104	(8)
C(6)	1.23770	1.27135	.16457	(1)
C(7)	1.54832	.00000	.96334	(1)
C(8)	1.23770	-1.27135	.16457	(1)
C(9)	.00000	.00000	-1.44025	(1)
H(10)	-2.07928	-1.45931	-.54020	(5)
H(11)	-1.20914	-2.15397	.84146	(5)
H(12)	-.98042	.00000	1.91703	(5)
H(13)	-2.62074	.00000	1.26547	(5)
H(14)	-2.07928	1.45931	-.54020	(5)
H(15)	-1.20914	2.15397	.84146	(5)
H(16)	2.07928	1.45931	-.54020	(5)
H(17)	1.20914	2.15397	.84146	(5)
H(18)	.98042	.00000	1.91703	(5)
H(19)	2.62074	.00000	1.26547	(5)
H(20)	2.07928	-1.45931	-.54020	(5)
H(21)	1.20914	-2.15397	.84146	(5)
H(22)	-.88684	.00000	-2.11032	(5)
H(23)	.88684	.00000	-2.11032	(5)

2-methyl-2-azabicyclo[2.2.2]octane, **4**

FINAL STERIC ENERGY IS 29.6240 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	-1.11421	.87350	-1.15294	(1)
C(2)	-.16071	-.25905	-1.60200	(1)
C(3)	.36406	-1.01377	-.37031	(1)
C(4)	-.82839	-1.48619	.47625	(1)
C(5)	-1.59700	-.26045	1.02399	(1)
C(6)	-1.03350	1.01485	.37664	(1)
C(7)	.44961	1.13983	.74896	(1)
N(8)	1.15415	-.11960	.48327	(8)
C(9)	2.53743	.07574	.06645	(1)
H(10)	-2.16065	.64679	-1.46011	(5)
H(11)	-.83321	1.83102	-1.64812	(5)
H(12)	-.69888	-.96066	-2.27906	(5)
H(13)	.68618	.15885	-2.19082	(5)
H(14)	.97798	-1.89194	-.67671	(5)
H(15)	-1.50392	-2.12018	-.14182	(5)
H(16)	-.47422	-2.12197	1.31961	(5)
H(17)	-1.49021	-.20115	2.13142	(5)
H(18)	-2.68555	-.35838	.80927	(5)
H(19)	-1.60272	1.91166	.71539	(5)
H(20)	.56216	1.40083	1.82631	(5)
H(21)	.90698	1.98014	.16199	(5)
H(22)	3.08469	.68604	.81710	(5)
H(23)	2.59887	.59624	-.92731	(5)
H(24)	3.06009	-.90130	-.01635	(5)

N-methyl-3-azabicyclo[3.2.2]nonane, **5**

FINAL STERIC ENERGY IS 30.8845 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	1.46410	.72708	-1.15838	(1)
C(2)	1.63348	-.79525	-.97599	(1)
C(3)	.65331	-1.37727	.04963	(1)
C(4)	.90539	-.72638	1.42291	(1)
C(5)	1.05837	.81381	1.33053	(1)
C(6)	.63758	1.38249	-.03494	(1)
C(7)	-.87665	1.23950	-.27761	(1)
N(8)	-1.45694	-.02202	.17386	(8)
C(9)	-.81471	-1.20427	-.39475	(1)
C(10)	-2.89906	-.04158	-.06075	(1)
H(11)	.99432	.94120	-2.14529	(5)
H(12)	2.47429	1.19774	-1.19539	(5)
H(13)	1.51700	-1.31085	-1.95678	(5)
H(14)	2.67409	-1.00928	-.63735	(5)
H(15)	.85828	-2.47292	.13401	(5)
H(16)	.07827	-.99064	2.12097	(5)

H(17)	1.83162	-1.15529	1.87138	(5)
H(18)	2.12478	1.08279	1.51449	(5)
H(19)	.47202	1.30186	2.14260	(5)
H(20)	.87138	2.47610	-.04674	(5)
H(21)	-1.10370	1.40192	-1.36770	(5)
H(22)	-1.38457	2.06831	.26671	(5)
H(23)	-.89014	-1.19356	-1.51699	(5)
H(24)	-1.37501	-2.10566	-.05515	(5)
H(25)	-3.38798	.82750	.42995	(5)
H(26)	-3.13547	-.00884	-1.15959	(5)
H(27)	-3.35337	-.96047	.36843	(5)

1-azabicyclo[3.2.2]nonane, **6**

FINAL STERIC ENERGY IS 30.8569 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	-1.29412	.73758	.97996	(1)
C(2)	-1.16968	-.79795	1.01094	(1)
N(3)	-.23986	-1.32331	.01651	(8)
C(4)	1.17478	-1.24069	.37766	(1)
C(5)	1.87335	.06886	.00644	(1)
C(6)	1.11413	1.33780	.40455	(1)
C(7)	-.36158	1.38645	-.05382	(1)
C(8)	-.57399	.70728	-1.41940	(1)
C(9)	-.55576	-.83906	-1.32433	(1)
H(10)	-1.09961	1.15863	1.99222	(5)
H(11)	-2.34709	1.00931	.73449	(5)
H(12)	-.87230	-1.14038	2.02691	(5)
H(13)	-2.17328	-1.24481	.82947	(5)
H(14)	1.29149	-1.42979	1.46879	(5)
H(15)	1.71232	-2.07681	-.12591	(5)
H(16)	2.05694	.08532	-1.09200	(5)
H(17)	2.88537	.08679	.47380	(5)
H(18)	1.16563	1.47017	1.50936	(5)
H(19)	1.65178	2.21329	-.03025	(5)
H(20)	-.64888	2.46345	-.14446	(5)
H(21)	-1.55634	1.02944	-1.83614	(5)
H(22)	.19302	1.06233	-2.14392	(5)
H(23)	.16248	-1.26555	-2.05927	(5)
H(24)	-1.55516	-1.23199	-1.61811	(5)

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exo-2-methyl-2-azabicyclo[2.2.1]heptane, **7**

FINAL STERIC ENERGY IS 44.7498 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	-1.81699	.19906	-.53080	(1)
C(2)	-1.15275	-1.20935	-.49181	(1)
C(3)	.11219	-.97386	.36013	(1)

C(4)	-.39573	.05536	1.37604	(1)
C(5)	-.84830	1.06314	.31119	(1)
C(6)	.46244	1.22110	-.48366	(1)
N(7)	1.00619	-.15616	-.48579	(8)
C(8)	2.40010	-.20132	-.05916	(1)
H(9)	-2.82777	.17128	-.06415	(5)
H(10)	-1.92246	.58544	-1.56865	(5)
H(11)	-1.82585	-1.94899	-.00270	(5)
H(12)	-.90224	-1.58373	-1.50906	(5)
H(13)	.58291	-1.89632	.76008	(5)
H(14)	-1.23539	-.32732	1.99641	(5)
H(15)	.40164	.45312	2.04046	(5)
H(16)	-1.28067	2.01114	.69369	(5)
H(17)	.29176	1.58496	-1.52338	(5)
H(18)	1.15129	1.93579	.03537	(5)
H(19)	3.02902	.42547	-.72781	(5)
H(20)	2.52401	.16542	.99581	(5)
H(21)	2.78636	-1.24182	-.11479	(5)

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endo-2-methyl-2-azabicyclo[2.2.1]heptane, **8**

FINAL STERIC ENERGY IS 45.5140 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	1.40649	.36601	-1.01541	(1)
C(2)	.57003	1.44871	-.27044	(1)
C(3)	-.09744	.65448	.87354	(1)
C(4)	1.00364	-.35742	1.21381	(1)
C(5)	1.09749	-.92064	-.21324	(1)
C(6)	-.37944	-1.28505	-.48307	(1)
N(7)	-1.09418	-.27130	.31344	(8)
C(8)	-2.28610	.29501	-.29905	(1)
H(9)	2.49289	.60685	-.97052	(5)
H(10)	1.11568	.27203	-2.08495	(5)
H(11)	1.23833	2.23671	.14454	(5)
H(12)	-.16613	1.94720	-.93591	(5)
H(13)	-.48479	1.25589	1.72068	(5)
H(14)	1.94641	.12270	1.55584	(5)
H(15)	.68114	-1.11825	1.95860	(5)
H(16)	1.82065	-1.74878	-.36455	(5)
H(17)	-.63127	-1.22561	-1.57184	(5)
H(18)	-.62692	-2.30681	-.11049	(5)
H(19)	-3.01959	-.50923	-.52292	(5)
H(20)	-2.77145	1.01576	.39361	(5)
H(21)	-2.04557	.82627	-1.25854	(5)

1,6-diazabicyclo[4.3.1]decane, conformer **9a**

FINAL STERIC ENERGY IS 34.1493 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE

N(1)	-.26314	-1.21158	-.51108	(8)
C(2)	-1.60940	-1.27235	.05957	(1)
C(3)	-1.97868	.00000	.83723	(1)
C(4)	-1.60940	1.27235	.05957	(1)
N(5)	-.26314	1.21158	-.51108	(8)
C(6)	.79240	1.42414	.48687	(1)
C(7)	2.14394	.77782	.15293	(1)
C(8)	2.14394	-.77782	.15293	(1)
C(9)	.79240	-1.42414	.48687	(1)
C(10)	-.13480	.00000	-1.30750	(1)
H(11)	-2.34127	-1.41253	-.76778	(5)
H(12)	-1.70917	-2.16995	.70992	(5)
H(13)	-1.46679	.00000	1.82493	(5)
H(14)	-3.06948	.00000	1.06328	(5)
H(15)	-2.34127	1.41253	-.76778	(5)
H(16)	-1.70917	2.16995	.70992	(5)
H(17)	.93799	2.52301	.60151	(5)
H(18)	.46223	1.06704	1.49656	(5)
H(19)	2.89348	1.12801	.90079	(5)
H(20)	2.50813	1.15743	-.82908	(5)
H(21)	2.50813	-1.15743	-.82908	(5)
H(22)	2.89348	-1.12801	.90079	(5)
H(23)	.46223	-1.06704	1.49656	(5)
H(24)	.93799	-2.52302	.60151	(5)
H(25)	.82391	.00000	-1.86368	(5)
H(26)	-.91312	.00000	-2.10186	(5)

1,6-diazabicyclo[4.3.1]decane, conformer **9b**

FINAL STERIC ENERGY IS 32.2472 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
N(1)	.35800	-1.23194	.56894	(8)
C(2)	1.56931	-1.21308	-.24725	(1)
C(3)	1.65582	.05193	-1.09892	(1)
C(4)	1.45304	1.29144	-.22549	(1)
N(5)	.29656	1.19241	.66483	(8)
C(6)	-.98916	1.63547	.13680	(1)
C(7)	-1.70607	.67972	-.81893	(1)
C(8)	-2.03177	-.68596	-.20330	(1)
C(9)	-.85739	-1.66739	-.12970	(1)
C(10)	.27332	-.05397	1.42343	(1)
H(11)	2.45564	-1.25876	.42495	(5)
H(12)	1.62470	-2.12365	-.88401	(5)
H(13)	.89476	.01889	-1.90764	(5)
H(14)	2.64547	.10247	-1.60761	(5)
H(15)	2.36282	1.43150	.40166	(5)
H(16)	1.37719	2.20419	-.85748	(5)
H(17)	-1.66530	1.84134	.99727	(5)
H(18)	-.85384	2.61949	-.36601	(5)
H(19)	-1.12374	.54737	-1.75558	(5)
H(20)	-2.66337	1.16062	-1.13026	(5)
H(21)	-2.47457	-.54267	.80810	(5)
H(22)	-2.83647	-1.16138	-.81254	(5)

H(23)	-.59787	-1.98414	-1.17013	(5)
H(24)	-1.21894	-2.59739	.37516	(5)
H(25)	-.62510	-.10463	2.07398	(5)
H(26)	1.13995	-.05866	2.12040	(5)

1,8-diazabicyclo[6.3.1]dodecane, conformer **10a**

FINAL STERIC ENERGY IS 39.1749 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	1.12843	-1.66817	-.63780	(1)
C(2)	2.21075	-.65252	-1.01177	(1)
C(3)	2.55295	.24778	.17622	(1)
N(4)	1.37317	.77774	.86024	(8)
C(5)	.46429	-.30026	1.21909	(1)
N(6)	.01220	-.99215	.01600	(8)
C(7)	.72348	1.94319	.24401	(1)
C(8)	-.40853	1.69942	-.78024	(1)
C(9)	-1.82476	1.52367	-.15835	(1)
C(10)	-2.60094	.23619	-.53485	(1)
C(11)	-2.43486	-.95823	.43074	(1)
C(12)	-1.17930	-1.80861	.19236	(1)
H(13)	.77745	-2.18061	-1.56139	(5)
H(14)	1.55195	-2.46091	.04000	(5)
H(15)	3.12399	-1.17993	-1.36988	(5)
H(16)	1.85797	-.02657	-1.86210	(5)
H(17)	3.14527	-.34571	.90915	(5)
H(18)	3.21857	1.07939	-.14469	(5)
H(19)	.97538	-1.02098	1.91400	(5)
H(20)	-.38981	.11758	1.78908	(5)
H(21)	.31515	2.58007	1.06159	(5)
H(22)	1.50823	2.57325	-.23481	(5)
H(23)	-.45105	2.59128	-1.44949	(5)
H(24)	-.16471	.85839	-1.46037	(5)
H(25)	-1.78155	1.62144	.94829	(5)
H(26)	-2.43935	2.39428	-.49077	(5)
H(27)	-3.68665	.49580	-.55313	(5)
H(28)	-2.35288	-.07337	-1.57509	(5)
H(29)	-2.46045	-.59251	1.48143	(5)
H(30)	-3.32371	-1.62454	.33017	(5)
H(31)	-1.34707	-2.40922	-.73096	(5)
H(32)	-1.03057	-2.54306	1.03155	(5)

1,8-diazabicyclo[6.3.1]dodecane, conformer **10b**

FINAL STERIC ENERGY IS 39.4929 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	-1.67072	1.45193	-.48856	(1)
C(2)	-2.42203	.20300	-.97494	(1)

C(3)	-2.38979	-.94852	.04740	(1)
N(4)	-1.07775	-1.14936	.67310	(8)
C(5)	-.65031	.13505	1.20829	(1)
N(6)	-.40416	1.04775	.10374	(8)
C(7)	-.08899	-1.70476	-.26616	(1)
C(8)	1.35023	-1.83121	.30278	(1)
C(9)	2.44848	-1.08709	-.48598	(1)
C(10)	2.25520	.40964	-.81572	(1)
C(11)	2.02078	1.36918	.38417	(1)
C(12)	.63305	2.03969	.34503	(1)
H(13)	-1.49070	2.13415	-1.34892	(5)
H(14)	-2.28701	2.01979	.26255	(5)
H(15)	-3.47620	.46519	-1.22074	(5)
H(16)	-1.96265	-.14424	-1.92861	(5)
H(17)	-3.13352	-.73344	.84786	(5)
H(18)	-2.72933	-1.89422	-.43099	(5)
H(19)	-1.42490	.55278	1.90677	(5)
H(20)	.25498	.00640	1.83207	(5)
H(21)	-.43209	-2.71810	-.57509	(5)
H(22)	-.05940	-1.10289	-1.21219	(5)
H(23)	1.38840	-1.52768	1.36947	(5)
H(24)	1.61923	-2.91376	.31981	(5)
H(25)	2.60161	-1.62895	-1.44957	(5)
H(26)	3.40848	-1.19707	.07182	(5)
H(27)	3.16708	.75653	-1.35756	(5)
H(28)	1.43113	.52324	-1.55444	(5)
H(29)	2.16720	.82017	1.33953	(5)
H(30)	2.80102	2.16515	.37818	(5)
H(31)	.62747	2.78430	-.48334	(5)
H(32)	.42630	2.60470	1.29513	(5)

1,8-diazabicyclo[6.3.1]dodecane, conformer **10c**

FINAL STERIC ENERGY IS 39.7359 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	1.68030	1.49124	.39442	(1)
C(2)	2.55458	.27446	.72987	(1)
C(3)	2.38869	-.86600	-.28879	(1)
N(4)	.99059	-1.12335	-.65390	(8)
C(5)	.43518	.14167	-1.11038	(1)
N(6)	.33986	1.05521	.01862	(8)
C(7)	.23802	-1.68524	.47936	(1)
C(8)	-1.21526	-2.12265	.22989	(1)
C(9)	-2.29148	-1.08995	-.16799	(1)
C(10)	-2.35477	.23805	.64518	(1)
C(11)	-2.10364	1.52425	-.18965	(1)
C(12)	-.67106	2.09336	-.10938	(1)
H(13)	1.62911	2.16350	1.27975	(5)
H(14)	2.14256	2.08437	-.44331	(5)
H(15)	3.62409	.57939	.79030	(5)
H(16)	2.28460	-.09769	1.74447	(5)
H(17)	2.95662	-.60848	-1.21135	(5)

H(18)	2.85805	-1.79713	.09975	(5)
H(19)	1.06449	.58212	-1.93078	(5)
H(20)	-.55030	-.03230	-1.57445	(5)
H(21)	.78638	-2.58931	.83330	(5)
H(22)	.25229	-.97844	1.35213	(5)
H(23)	-1.20566	-2.92596	-.54388	(5)
H(24)	-1.57079	-2.62014	1.16383	(5)
H(25)	-2.23034	-.87852	-1.25624	(5)
H(26)	-3.28171	-1.59420	-.05894	(5)
H(27)	-3.37625	.31452	1.08780	(5)
H(28)	-1.66659	.20176	1.51732	(5)
H(29)	-2.37651	1.33813	-1.25249	(5)
H(30)	-2.80767	2.31825	.15323	(5)
H(31)	-.61447	2.75390	.78571	(5)
H(32)	-.45478	2.74247	-1.00295	(5)

1,8-diazabicyclo[6.3.1]dodecane, conformer **10d**

FINAL STERIC ENERGY IS 39.8749 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	1.19541	1.65044	.62804	(1)
C(2)	2.27744	.62460	.99389	(1)
C(3)	2.57452	-.34740	-.16020	(1)
N(4)	1.35854	-.85742	-.79825	(8)
C(5)	.54044	.27593	-1.19517	(1)
N(6)	.06826	.98220	-.01323	(8)
C(7)	.67433	-1.88474	.01157	(1)
C(8)	-.86934	-1.96894	-.08326	(1)
C(9)	-1.60507	-1.08252	.96259	(1)
C(10)	-2.72692	-.16459	.43789	(1)
C(11)	-2.35302	.92433	-.58819	(1)
C(12)	-1.12908	1.78520	-.22918	(1)
H(13)	.85440	2.17063	1.55084	(5)
H(14)	1.61937	2.43729	-.05629	(5)
H(15)	3.21106	1.14881	1.30051	(5)
H(16)	1.94033	.04858	1.88544	(5)
H(17)	3.18398	.18256	-.92673	(5)
H(18)	3.20361	-1.19395	.19510	(5)
H(19)	1.12487	.96762	-1.86115	(5)
H(20)	-.29647	-.08378	-1.82231	(5)
H(21)	1.09590	-2.87221	-.28947	(5)
H(22)	.94951	-1.77346	1.09284	(5)
H(23)	-1.22515	-1.76153	-1.11378	(5)
H(24)	-1.16769	-3.02681	.10744	(5)
H(25)	-2.05274	-1.76196	1.72661	(5)
H(26)	-.87383	-.47455	1.53747	(5)
H(27)	-3.53081	-.80221	.00067	(5)
H(28)	-3.19059	.34172	1.31773	(5)
H(29)	-2.21379	.45436	-1.58584	(5)
H(30)	-3.23065	1.60103	-.71445	(5)
H(31)	-1.36249	2.35053	.70129	(5)
H(32)	-.93956	2.54845	-1.03453	(5)

1,8-diazabicyclo[6.3.1]dodecane, conformer **10e**

FINAL STERIC ENERGY IS 40.5185 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	1.40874	1.64159	.45263	(1)
C(2)	2.45040	.57495	.81550	(1)
C(3)	2.53852	-.53433	-.24459	(1)
N(4)	1.22539	-1.00189	-.69559	(8)
C(5)	.45122	.15194	-1.11516	(1)
N(6)	.16156	1.01267	.02580	(8)
C(7)	.54399	-1.81435	.31877	(1)
C(8)	-.94202	-2.14432	.04629	(1)
C(9)	-1.96008	-1.16573	.69426	(1)
C(10)	-2.62671	-.09665	-.22013	(1)
C(11)	-2.30984	1.36653	.15230	(1)
C(12)	-.93805	1.93448	-.25392	(1)
H(13)	1.80643	2.30829	-.36291	(5)
H(14)	1.22285	2.28744	1.33985	(5)
H(15)	3.44860	1.04957	.95309	(5)
H(16)	2.18519	.12799	1.80036	(5)
H(17)	3.13649	-1.39026	.14050	(5)
H(18)	3.09870	-.14488	-1.12462	(5)
H(19)	-.47673	-.19419	-1.60547	(5)
H(20)	1.00435	.72073	-1.91200	(5)
H(21)	.62329	-1.33225	1.32945	(5)
H(22)	1.09996	-2.77583	.40635	(5)
H(23)	-1.13402	-2.26454	-1.04222	(5)
H(24)	-1.13656	-3.15264	.48385	(5)
H(25)	-1.49584	-.66997	1.57547	(5)
H(26)	-2.78320	-1.78508	1.12479	(5)
H(27)	-2.41796	-.28680	-1.29368	(5)
H(28)	-3.73177	-.22659	-.12753	(5)
H(29)	-2.42708	1.47634	1.25547	(5)
H(30)	-3.09443	2.02189	-.29409	(5)
H(31)	-.93834	2.21800	-1.34133	(5)
H(32)	-.78295	2.88562	.30940	(5)

1,8-diazabicyclo[6.3.1]dodecane, conformer **10f**

FINAL STERIC ENERGY IS 40.9988 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	-2.20520	-1.18138	.03675	(1)
N(2)	-.82729	-1.20543	.52838	(8)
C(3)	-.52647	.03806	1.23296	(1)
C(4)	-2.49686	.06461	-.80197	(1)
C(5)	-2.07756	1.32600	-.04408	(1)
N(6)	-.69821	1.25491	.44292	(8)

C(7)	.28545	1.54963	-.60120	(1)
C(8)	1.72912	1.78349	-.13867	(1)
C(9)	2.56342	.59872	.38078	(1)
C(10)	2.53850	-.68889	-.47404	(1)
C(11)	1.59258	-1.81653	-.00721	(1)
C(12)	.12193	-1.71722	-.46308	(1)
H(13)	-2.42727	-2.10368	-.54488	(5)
H(14)	-2.89651	-1.19865	.90947	(5)
H(15)	-1.19857	.10400	2.11702	(5)
H(16)	.48239	-.00451	1.67348	(5)
H(17)	-1.95884	.00684	-1.77428	(5)
H(18)	-3.58229	.11170	-1.04772	(5)
H(19)	-2.21942	2.22691	-.68132	(5)
H(20)	-2.75696	1.46450	.82720	(5)
H(21)	.26418	.77318	-1.40521	(5)
H(22)	-.03447	2.48942	-1.10913	(5)
H(23)	2.28430	2.21858	-1.00395	(5)
H(24)	1.72563	2.58191	.63976	(5)
H(25)	3.62260	.95008	.42575	(5)
H(26)	2.31870	.36493	1.43751	(5)
H(27)	2.34222	-.43711	-1.54021	(5)
H(28)	3.57329	-1.10877	-.46209	(5)
H(29)	1.99889	-2.76853	-.42587	(5)
H(30)	1.65107	-1.94307	1.09661	(5)
H(31)	.05431	-1.14753	-1.42439	(5)
H(32)	-.20497	-2.74951	-.72740	(5)

1,8-diazabicyclo[6.3.1]dodecane, conformer **10g**

FINAL STERIC ENERGY IS 42.5606 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	1.51875	-1.60876	-.50791	(1)
C(2)	2.68753	-.61090	-.39495	(1)
C(3)	2.16522	.82486	-.38389	(1)
N(4)	1.19204	1.05627	.69348	(8)
C(5)	.53812	-.17684	1.11916	(1)
N(6)	.26613	-1.01152	-.04187	(8)
C(7)	.24700	2.12681	.36399	(1)
C(8)	-.84190	1.77903	-.67990	(1)
C(9)	-2.17011	1.21933	-.09982	(1)
C(10)	-2.57991	-.20243	-.56283	(1)
C(11)	-2.18431	-1.35864	.38164	(1)
C(12)	-.80514	-1.98422	.12614	(1)
H(13)	1.39481	-1.92314	-1.56857	(5)
H(14)	1.76025	-2.53465	.08393	(5)
H(15)	3.25772	-.80069	.54340	(5)
H(16)	3.40401	-.76078	-1.23411	(5)
H(17)	3.01090	1.54076	-.27130	(5)
H(18)	1.70382	1.03654	-1.38503	(5)
H(19)	1.19529	-.72783	1.84616	(5)
H(20)	-.38805	.06557	1.68046	(5)
H(21)	-.24231	2.47778	1.29949	(5)
H(22)	.82821	3.00474	-.00051	(5)

H(23)	-1.08898	2.71805	-1.22963	(5)
H(24)	-.44479	1.09299	-1.45763	(5)
H(25)	-2.16785	1.27097	1.01072	(5)
H(26)	-2.98382	1.91769	-.41043	(5)
H(27)	-3.69321	-.21373	-.64702	(5)
H(28)	-2.20591	-.40123	-1.59210	(5)
H(29)	-2.26486	-1.01991	1.43841	(5)
H(30)	-2.94393	-2.16958	.28096	(5)
H(31)	-.87463	-2.59794	-.80118	(5)
H(32)	-.55185	-2.69538	.96172	(5)

GG'G' DEAP

FINAL STERIC ENERGY IS 19.1829 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
N(1)	-.25032	.00806	.18230	(8)
C(2)	-.76404	-1.25098	-.37642	(1)
C(3)	-2.16004	-1.62100	.13566	(1)
C(4)	-.95579	1.17547	-.36491	(1)
C(5)	-.73352	2.47048	.42335	(1)
C(6)	1.21912	.13410	.14809	(1)
C(7)	1.85573	-.84276	1.14820	(1)
C(8)	1.80627	-.06044	-1.25679	(1)
H(9)	-.77433	-1.20255	-1.50048	(5)
H(10)	-.08534	-2.08865	-.10470	(5)
H(11)	-2.45383	-2.63965	-.20293	(5)
H(12)	-2.19798	-1.62206	1.24775	(5)
H(13)	-2.94862	-.92697	-.22604	(5)
H(14)	-2.05006	.97797	-.35909	(5)
H(15)	-.67612	1.33363	-1.44244	(5)
H(16)	-1.42256	3.27275	.07662	(5)
H(17)	.29705	2.87002	.30918	(5)
H(18)	-.92216	2.32440	1.51019	(5)
H(19)	1.49233	1.15663	.49614	(5)
H(20)	1.39384	-.75302	2.15664	(5)
H(21)	2.94251	-.63783	1.27136	(5)
H(22)	1.76876	-1.90469	.83442	(5)
H(23)	1.38677	.65855	-1.99320	(5)
H(24)	2.90783	.09606	-1.25316	(5)
H(25)	1.63182	-1.08432	-1.65245	(5)

AGA DEAP

FINAL STERIC ENERGY IS 19.9287 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
N(1)	.10978	-.14071	.33105	(8)
C(2)	.68514	1.19437	.55073	(1)
C(3)	.97507	2.01294	-.71195	(1)
C(4)	1.04816	-1.04625	-.34945	(1)

C(5)	2.40713	-1.20294	.34163	(1)
C(6)	-1.23132	-.12398	-.29267	(1)
C(7)	-2.18956	.80331	.47546	(1)
C(8)	-1.85080	-1.53336	-.29421	(1)
H(9)	.01757	1.78025	1.21752	(5)
H(10)	1.62325	1.09706	1.13806	(5)
H(11)	1.40158	3.00758	-.45257	(5)
H(12)	1.71161	1.51337	-1.37785	(5)
H(13)	.05829	2.20430	-1.31049	(5)
H(14)	1.20196	-.71894	-1.41471	(5)
H(15)	.60392	-2.06327	-.39853	(5)
H(16)	2.99750	-2.02553	-.12047	(5)
H(17)	2.29268	-1.44996	1.42056	(5)
H(18)	3.03245	-.28714	.26524	(5)
H(19)	-1.14936	.23508	-1.35814	(5)
H(20)	-1.92255	1.87691	.37133	(5)
H(21)	-2.21827	.56149	1.56117	(5)
H(22)	-3.23099	.71344	.09497	(5)
H(23)	-1.35015	-2.22230	-1.00775	(5)
H(24)	-1.81609	-2.00142	.71465	(5)
H(25)	-2.91907	-1.50557	-.60311	(5)

GAG' DEAP

FINAL STERIC ENERGY IS 20.4405 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
N(1)	-.12080	-.14727	.40658	(8)
C(2)	-.64667	-1.04924	-.62292	(1)
C(3)	-1.91142	-1.80234	-.20118	(1)
C(4)	-1.03261	.90344	.86955	(1)
C(5)	-1.35940	2.00329	-.14312	(1)
C(6)	1.28413	.27096	.25386	(1)
C(7)	1.64329	.67969	-1.18180	(1)
C(8)	2.19454	-.86893	.73129	(1)
H(9)	-.85057	-.47937	-1.57071	(5)
H(10)	.12533	-1.81022	-.87339	(5)
H(11)	-2.18876	-2.57330	-.95434	(5)
H(12)	-1.76997	-2.32790	.76935	(5)
H(13)	-2.78977	-1.12890	-.09760	(5)
H(14)	-.60669	1.37396	1.78415	(5)
H(15)	-1.98236	.43700	1.20956	(5)
H(16)	-2.12003	2.70625	.26409	(5)
H(17)	-1.77357	1.59403	-1.09006	(5)
H(18)	-.46731	2.61507	-.39714	(5)
H(19)	1.47051	1.14484	.92511	(5)
H(20)	.97845	1.47502	-1.57911	(5)
H(21)	1.59539	-.17531	-1.89047	(5)
H(22)	2.68127	1.07689	-1.23449	(5)
H(23)	1.94494	-1.18162	1.76968	(5)
H(24)	2.12243	-1.77181	.08736	(5)
H(25)	3.26289	-.55814	.73375	(5)

GGG'2 DEAP

FINAL STERIC ENERGY IS 20.6812 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
N(1)	-.12409	-.11056	-.21519	(8)
C(2)	-.44162	.94023	.76784	(1)
C(3)	-1.25169	2.08168	.14855	(1)
C(4)	-.97272	-1.30277	-.09729	(1)
C(5)	-2.45970	-1.04051	-.34738	(1)
C(6)	1.30360	-.44009	-.36131	(1)
C(7)	1.92651	-.96749	.93902	(1)
C(8)	2.07364	.77487	-.89835	(1)
H(9)	-.99462	.50491	1.64077	(5)
H(10)	.49220	1.37578	1.19448	(5)
H(11)	-1.46982	2.87513	.89761	(5)
H(12)	-.69960	2.56310	-.68891	(5)
H(13)	-2.22743	1.73774	-.25587	(5)
H(14)	-.84308	-1.77227	.91702	(5)
H(15)	-.63909	-2.06291	-.84026	(5)
H(16)	-3.03871	-1.99089	-.35401	(5)
H(17)	-2.62848	-.54830	-1.33083	(5)
H(18)	-2.91235	-.39716	.43794	(5)
H(19)	1.39459	-1.24069	-1.13445	(5)
H(20)	1.41880	-1.88635	1.30451	(5)
H(21)	1.89697	-.22301	1.76311	(5)
H(22)	2.99584	-1.23543	.78862	(5)
H(23)	1.60873	1.17362	-1.82741	(5)
H(24)	2.12802	1.61112	-.16914	(5)
H(25)	3.12275	.50483	-1.15234	(5)

GGG'1 DEAP

FINAL STERIC ENERGY IS 20.7664 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
N(1)	.11129	.05440	-.13882	(8)
C(2)	.36689	-1.30143	.36175	(1)
C(3)	1.76832	-1.82379	.03458	(1)
C(4)	.98140	1.07648	.47044	(1)
C(5)	2.06066	1.55486	-.50289	(1)
C(6)	-1.30074	.46741	-.19268	(1)
C(7)	-1.98470	.37501	1.17825	(1)
C(8)	-2.06082	-.35566	-1.24219	(1)
H(9)	.20374	-1.34110	1.47452	(5)
H(10)	-.36291	-2.00884	-.08822	(5)
H(11)	1.88365	-2.88589	.34625	(5)
H(12)	1.97579	-1.77896	-1.05765	(5)
H(13)	2.56566	-1.24972	.55438	(5)
H(14)	1.45562	.68353	1.40633	(5)
H(15)	.37994	1.96440	.78783	(5)
H(16)	2.70555	2.33521	-.04096	(5)

H(17)	1.61217	1.99770	-1.41986	(5)
H(18)	2.72833	.72817	-.82835	(5)
H(19)	-1.33654	1.53021	-.53461	(5)
H(20)	-1.44401	.95379	1.95865	(5)
H(21)	-2.06648	-.67338	1.53870	(5)
H(22)	-3.01986	.78070	1.13671	(5)
H(23)	-1.53440	-.35411	-2.22259	(5)
H(24)	-2.20362	-1.41513	-.94004	(5)
H(25)	-3.07668	.06243	-1.41948	(5)

AGG' DEAP

FINAL STERIC ENERGY IS 21.1165 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
N(1)	-.13562	-.33912	-.28504	(8)
C(2)	-.42589	.98370	-.85333	(1)
C(3)	-.82131	2.08482	.13727	(1)
C(4)	-1.17955	-.88921	.58609	(1)
C(5)	-2.54579	-1.01886	-.09338	(1)
C(6)	1.23490	-.63691	.16456	(1)
C(7)	1.70699	.26291	1.31127	(1)
C(8)	2.21165	-.57100	-1.01805	(1)
H(9)	.44294	1.33405	-1.45040	(5)
H(10)	-1.24932	.87282	-1.59392	(5)
H(11)	-.99544	3.04906	-.39048	(5)
H(12)	-1.76224	1.84694	.67877	(5)
H(13)	-.04134	2.27832	.90194	(5)
H(14)	-1.27336	-.26989	1.51973	(5)
H(15)	-.87755	-1.90782	.92057	(5)
H(16)	-3.27597	-1.53538	.56881	(5)
H(17)	-2.47916	-1.61123	-1.03296	(5)
H(18)	-2.98861	-.03212	-.34922	(5)
H(19)	1.25249	-1.69195	.53074	(5)
H(20)	.98776	.27651	2.15903	(5)
H(21)	1.86960	1.31128	.98193	(5)
H(22)	2.67845	-.09215	1.72148	(5)
H(23)	1.85329	-1.17766	-1.87935	(5)
H(24)	2.37670	.46532	-1.38298	(5)
H(25)	3.21109	-.96987	-.73475	(5)

AG'A DEAP

FINAL STERIC ENERGY IS 21.4209 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
C(1)	1.27770	1.84688	.48875	(1)
C(2)	.24275	1.05550	-.32871	(1)
C(3)	-1.02855	1.91283	-.43305	(1)
N(4)	-.04923	-.24377	.30825	(8)
C(5)	-1.09022	-1.03891	-.37039	(1)

C(6)	-2.43590	-.97716	.35703	(1)
C(7)	1.12648	-1.06776	.61575	(1)
C(8)	1.96532	-1.48789	-.59661	(1)
H(9)	1.41087	2.87484	.08491	(5)
H(10)	2.28555	1.37928	.47053	(5)
H(11)	.97105	1.95224	1.55311	(5)
H(12)	.64841	.88337	-1.36652	(5)
H(13)	-.80228	2.92085	-.84578	(5)
H(14)	-1.50394	2.06891	.56051	(5)
H(15)	-1.78981	1.46882	-1.10957	(5)
H(16)	-.78627	-2.11394	-.41751	(5)
H(17)	-1.20350	-.71399	-1.43690	(5)
H(18)	-3.19905	-1.60693	-.15220	(5)
H(19)	-2.84743	.05286	.40916	(5)
H(20)	-2.34768	-1.34890	1.40210	(5)
H(21)	1.77518	-.53380	1.34285	(5)
H(22)	.79468	-1.98096	1.16009	(5)
H(23)	2.80430	-2.15206	-.29100	(5)
H(24)	1.36815	-2.04690	-1.34952	(5)
H(25)	2.42016	-.61612	-1.11502	(5)

GGA DEAP

FINAL STERIC ENERGY IS 21.5169 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
N(1)	.10867	.08498	-.00270	(8)
C(2)	.83269	1.33541	-.27031	(1)
C(3)	2.24831	1.36773	.31720	(1)
C(4)	.79421	-1.06155	-.63591	(1)
C(5)	1.34639	-2.03691	.40577	(1)
C(6)	-1.32852	.12685	-.34293	(1)
C(7)	-2.02844	1.34760	.27976	(1)
C(8)	-2.02876	-1.13220	.20077	(1)
H(9)	.86812	1.53413	-1.37813	(5)
H(10)	.28678	2.18822	.18616	(5)
H(11)	2.71692	2.36751	.17775	(5)
H(12)	2.23907	1.16161	1.41064	(5)
H(13)	2.92977	.62875	-.15602	(5)
H(14)	1.62994	-.71096	-1.29202	(5)
H(15)	.10584	-1.60662	-1.32789	(5)
H(16)	1.86153	-2.89688	-.07714	(5)
H(17)	.54029	-2.45430	1.04818	(5)
H(18)	2.08382	-1.54686	1.07870	(5)
H(19)	-1.45010	.17263	-1.46347	(5)
H(20)	-1.73891	2.30222	-.21027	(5)
H(21)	-1.81450	1.43957	1.36783	(5)
H(22)	-3.13337	1.27725	.17145	(5)
H(23)	-1.66683	-2.07155	-.26803	(5)
H(24)	-1.88930	-1.23538	1.29980	(5)
H(25)	-3.12481	-1.09813	.01349	(5)

G'G'G' DEAP

FINAL STERIC ENERGY IS 21.7420 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
N(1)	.26720	-.38398	-.15161	(8)
C(2)	-.68458	-1.39841	.32754	(1)
C(3)	-2.05239	-1.41971	-.35837	(1)
C(4)	1.61233	-.66987	.37306	(1)
C(5)	2.74539	-.05028	-.45286	(1)
C(6)	-.10221	1.03872	.00772	(1)
C(7)	-.72030	1.35608	1.37565	(1)
C(8)	-1.00572	1.49932	-1.14367	(1)
H(9)	-.23817	-2.40581	.15870	(5)
H(10)	-.81910	-1.31066	1.44090	(5)
H(11)	-2.61120	-2.34733	-.10139	(5)
H(12)	-2.69920	-.57383	-.04439	(5)
H(13)	-1.95811	-1.39518	-1.46665	(5)
H(14)	1.78218	-1.77137	.37461	(5)
H(15)	1.69180	-.34096	1.44563	(5)
H(16)	3.73781	-.41899	-.10965	(5)
H(17)	2.77893	1.05768	-.38110	(5)
H(18)	2.65374	-.31369	-1.53007	(5)
H(19)	.82707	1.65034	-.07912	(5)
H(20)	-.06350	1.04096	2.21575	(5)
H(21)	-1.70809	.86930	1.52153	(5)
H(22)	-.88623	2.44996	1.49357	(5)
H(23)	-.58720	1.20700	-2.13240	(5)
H(24)	-2.03498	1.09305	-1.08452	(5)
H(25)	-1.10773	2.60740	-1.15190	(5)

G'GG' DEAP

FINAL STERIC ENERGY IS 21.7512 KCAL.

FINAL ATOMIC COORDINATE

ATOM	X	Y	Z	TYPE
N(1)	-.33581	-.06166	-.23595	(8)
C(2)	-.29451	1.21517	.49393	(1)
C(3)	.76275	2.22459	.04103	(1)
C(4)	-1.54065	-.83225	.11419	(1)
C(5)	-2.85722	-.17777	-.31950	(1)
C(6)	.86560	-.92314	-.18820	(1)
C(7)	1.44376	-1.07428	1.22457	(1)
C(8)	1.92887	-.44926	-1.18823	(1)
H(9)	-1.27528	1.72452	.37097	(5)
H(10)	-.18828	1.02851	1.59815	(5)
H(11)	.55858	3.23189	.46826	(5)
H(12)	1.78394	1.94976	.37887	(5)
H(13)	.77707	2.33957	-1.06544	(5)
H(14)	-1.56556	-1.03441	1.22094	(5)
H(15)	-1.49937	-1.82729	-.38527	(5)
H(16)	-3.71127	-.88126	-.19944	(5)
H(17)	-2.83023	.12344	-1.39035	(5)

H(18)	-3.10732	.72375	.27996	(5)
H(19)	.57002	-1.94402	-.53590	(5)
H(20)	.68593	-1.44345	1.94975	(5)
H(21)	1.85187	-.12036	1.62192	(5)
H(22)	2.28096	-1.80705	1.23651	(5)
H(23)	1.48719	-.24594	-2.18908	(5)
H(24)	2.46086	.46706	-.86445	(5)
H(25)	2.71210	-1.22625	-1.33409	(5)

Selected portions of Gaussian Output for endo 2-methyl-2-azabicyclo[2.2.1]heptane

```
*********************************************
 Gaussian 94:  x86-Windows-G94RevD.3  1-May-1996
                12-Feb-1998
 *********************************************
 Default route:  MaxDisk=13107200
 ------------------------------
 # HF/3-21g/b3lyp extrabasis nmr
 ------------------------------
 1/38=1/1;
 2/12=2,17=6,18=5/2;
 3/5=5,10=1,11=2,25=1,30=1/1,2,8,3;
 4//1;
 5/5=2,38=4,42=-5/2;
 8/6=1,11=11,27=13107200/1;
 10/13=100/2;
 6/7=2,8=2,9=2,10=2,19=1,28=1/1;
 99/5=1,9=1/99;
 ---------------------------------------------
 endo 2-methyl-2-azabicyclo2.2.1heptane bdif//mm3
 ---------------------------------------------
 Symbolic Z-matrix:
    Charge = 0 Multiplicity = 1
 C      0      0.          0.          0.
 C      1      1.55783
 C      1      1.54737   2      102.86985
 H      1      1.11367   2      110.74425 3     -118.325890
 H      1      1.11231   2      112.22175 3     120.66225 0
 C      2      1.54436   1      103.23228 3     0.71674   0
 C      3      1.53708   1      100.8863  2     -36.10167 0
 C      3      1.54495   1      107.24945 2     69.12117  0
 H      2      1.11346   1      110.35597 3     118.60491 0
 H      2      1.11058   1      112.41434 3     -121.178930
 H      3      1.10988   1      114.81321 2     -161.712320
 N      6      1.47107   2      109.5367  1     -68.76984 0
 H      6      1.10872   2      115.97642 1     161.45512 0
 H      7      1.1119    3      113.08138 1     -60.64056 0
 H      7      1.11252   3      112.87098 1     174.24515 0
 H      8      1.11912   3      111.8665  1     46.14209  0
 H      8      1.11533   3      111.71046 1     168.50805 0
 C      12     1.45469   6      118.06525 2     -67.72048 0
 H      18     1.11132   12     110.12017 6     -170.621540
 H      18     1.11135   12     110.3596  6     -51.66351 0
 H      18     1.12281   12     111.6276  6     69.23172  0
 ---------------------------------------------------------------
```

Z-Matrix orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.557828
3	6	1.508495	0.000000	-0.344656
4	1	-0.494165	0.916771	-0.394460
5	1	-0.525120	-0.885731	-0.420666
6	6	1.503239	0.018806	1.911331
7	6	2.063139	0.889378	0.779614
8	6	2.072241	-1.378582	0.065937
9	1	-0.499797	0.916505	1.945147
10	1	-0.531522	-0.878376	1.981294
11	1	1.749511	0.316115	-1.380903
12	7	2.113152	-1.265952	1.535237
13	1	1.755681	0.338990	2.942358
14	1	1.640361	1.917731	0.770651
15	1	3.174365	0.943024	0.780120
16	1	1.415430	-2.216788	-0.278215
17	1	3.101328	-1.538968	-0.333079
18	6	1.717828	-2.454035	2.275713
19	1	2.372760	-3.309632	2.003584
20	1	1.820576	-2.280489	3.368608
21	1	0.655224	-2.743458	2.057037

```
Stoichiometry    C7H13N
 Framework group  C1[X(C7H13N)]
 Deg. of freedom   57
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
---------------------------------------------------------------
 Rotational constants (GHZ):      3.2453752      2.1017047
1.9140340
 Isotopes: C-12,C-12,C-12,H-1,H-1,C-12,C-12,C-12,H-1,H-1,H-1,N-14,H-
1,H-1,H-1,H-1
 ,H-1,C-12,H-1,H-1,H-1
 Standard basis: 3-21G (6D, 7F)
 There are   117 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant
integrals=1.000.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   117 basis functions      191 primitive gaussians
    31 alpha electrons       31 beta electrons
       nuclear repulsion energy       414.4209428027 Hartrees.
 One-electron integrals computed using PRISM.
 The smallest eigenvalue of the overlap matrix is  1.241D-04
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
```

```
SCF Done:  E(RB+HF-LYP) =  -327.824037404     A.U. after   15 cycles
             Convg  =    0.2444D-08             -V/T =  2.0090
             S**2   =    0.0000
Range of M.O.s used for correlation:     1   117
NBasis=   117 NAE=    31 NBE=    31 NFC=     0 NFV=     0
NROrb=    117 NOA=    31 NOB=    31 NVA=    86 NVB=    86

**** Warning!!: The largest alpha MO coeffient is  0.54712231D+02

        Differentiating once with respect to magnetic field using
GIAOs.
 Symmetry not used in FoFDir.
 MinBra= 0 MaxBra= 2 MinRaf= 0 MaxRaf= 2.
 IRaf=       0 NMat=   1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0
JSym2E=0.
         There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
 Inv2:  IOpt= 1 Iter= 1 AM= 7.20D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  18 with in-core refinement.
 Calculating GIAO nuclear magnetic shielding tensors.
 GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =   170.6669   Anisotropy =    23.4205
   XX=   163.5510   YX=     1.2178   ZX=    -3.9101
   XY=     8.6734   YY=   176.8556   ZY=   -16.0915
   XZ=     0.2732   YZ=    -5.1535   ZZ=   171.5940
   Eigenvalues:   161.2284   164.4916   186.2805
  2  C    Isotropic =   178.1743   Anisotropy =    21.0596
   XX=   166.4189   YX=    -0.5204   ZX=   -18.7103
   XY=    -0.5731   YY=   186.7043   ZY=     4.9428
   XZ=   -11.8096   YZ=     0.6788   ZZ=   181.3999
   Eigenvalues:   156.8748   185.4341   192.2141
  3  C    Isotropic =   163.9244   Anisotropy =    24.1452
   XX=   156.7382   YX=     2.2579   ZX=     4.1615
   XY=    -5.0594   YY=   163.4422   ZY=     3.7267
   XZ=   -12.6756   YZ=    18.2275   ZZ=   171.5929
   Eigenvalues:   154.6149   157.1372   180.0212
  4  H    Isotropic =    30.8268   Anisotropy =    11.7133
   XX=    36.8705   YX=     2.0737   ZX=    -3.8481
   XY=     3.0780   YY=    28.5390   ZY=    -0.6130
   XZ=    -3.0025   YZ=    -0.5554   ZZ=    27.0708
   Eigenvalues:    25.9687    27.8759    38.6356
  5  H    Isotropic =    31.2330   Anisotropy =     9.5972
   XX=    28.0040   YX=     0.0018   ZX=    -0.6965
   XY=    -0.2664   YY=    28.1615   ZY=    -0.6749
   XZ=    -1.0562   YZ=    -0.1699   ZZ=    37.5336
   Eigenvalues:    27.8316    28.2364    37.6312
  6  C    Isotropic =   145.0892   Anisotropy =    22.2446
   XX=   156.7722   YX=    -0.7831   ZX=    -0.4587
   XY=     5.2077   YY=   143.8631   ZY=    13.2315
   XZ=    15.0964   YZ=    -1.6287   ZZ=   134.6323
   Eigenvalues:   130.5437   144.8050   159.9190
```

```
 7  C    Isotropic =   162.6784   Anisotropy =    18.6881
  XX=   163.7011   YX=    -9.4806   ZX=     8.7459
  XY=   -10.3013   YY=   159.2056   ZY=    -2.7397
  XZ=     2.5775   YZ=    -2.0485   ZZ=   165.1284
  Eigenvalues:   151.0865   161.8115   175.1371
 8  C    Isotropic =   146.7930   Anisotropy =    25.5619
  XX=   153.3607   YX=    -8.0383   ZX=    -2.8468
  XY=   -11.7920   YY=   141.5081   ZY=     9.5407
  XZ=   -10.5342   YZ=     4.7586   ZZ=   145.5103
  Eigenvalues:   134.7027   141.8421   163.8343
 9  H    Isotropic =    31.2520   Anisotropy =    12.6065
  XX=    29.5372   YX=     4.5220   ZX=    -0.1600
  XY=     4.4966   YY=    37.1261   ZY=     2.6833
  XZ=    -0.2344   YZ=     2.6074   ZZ=    27.0927
  Eigenvalues:    25.7198    28.3798    39.6563
10  H    Isotropic =    30.3659   Anisotropy =     8.1962
  XX=    30.5665   YX=    -1.6204   ZX=     1.4619
  XY=    -2.3973   YY=    31.7081   ZY=    -3.9299
  XZ=     1.8452   YZ=    -4.1390   ZZ=    28.8231
  Eigenvalues:    25.9711    29.2966    35.8300
11  H    Isotropic =    30.6082   Anisotropy =    11.0153
  XX=    31.3184   YX=    -5.0439   ZX=    -1.0054
  XY=    -5.3580   YY=    33.2199   ZY=     1.0232
  XZ=    -1.9499   YZ=     1.8594   ZZ=    27.2862
  Eigenvalues:    26.7234    27.1494    37.9517
12  N    Isotropic =   216.7466   Anisotropy =    56.1999
  XX=   236.9293   YX=    -4.0840   ZX=    14.3770
  XY=    -0.7696   YY=   220.3282   ZY=    34.9231
  XZ=    15.4645   YZ=    49.8119   ZZ=   192.9821
  Eigenvalues:   159.7619   236.2647   254.2132
13  H    Isotropic =    29.5607   Anisotropy =     9.0288
  XX=    27.5947   YX=    -0.3933   ZX=    -1.8996
  XY=    -0.8856   YY=    28.8880   ZY=     4.6837
  XZ=    -2.0804   YZ=     3.7509   ZZ=    32.1996
  Eigenvalues:    25.7624    27.3398    35.5800
14  H    Isotropic =    31.1468   Anisotropy =    11.0407
  XX=    34.1136   YX=     1.3007   ZX=     5.6214
  XY=     1.3719   YY=    27.6474   ZY=     0.4696
  XZ=     5.0125   YZ=     0.3532   ZZ=    31.6793
  Eigenvalues:    26.9584    27.9746    38.5072
15  H    Isotropic =    30.4627   Anisotropy =    11.0253
  XX=    27.1806   YX=    -0.6608   ZX=     1.0594
  XY=     0.0993   YY=    29.3781   ZY=    -5.0009
  XZ=     0.7168   YZ=    -4.8553   ZZ=    34.8294
  Eigenvalues:    26.4094    27.1658    37.8129
16  H    Isotropic =    30.5491   Anisotropy =     7.4412
  XX=    29.4873   YX=     1.3243   ZX=     1.1386
  XY=     0.6203   YY=    29.5668   ZY=     3.8282
  XZ=     2.0755   YZ=     3.2411   ZZ=    32.5932
  Eigenvalues:    27.2321    28.9054    35.5099
17  H    Isotropic =    29.0851   Anisotropy =    11.0863
  XX=    26.4859   YX=     2.1548   ZX=    -0.9666
  XY=     2.2638   YY=    35.9826   ZY=     0.4930
  XZ=    -1.0120   YZ=     0.4168   ZZ=    24.7869
  Eigenvalues:    24.1646    26.6148    36.4760
18  C    Isotropic =   164.6984   Anisotropy =    50.3356
  XX=   185.1345   YX=   -22.6761   ZX=    10.2238
```

```
   XY=   -18.5765   YY=   151.8396   ZY=    -4.3552
   XZ=    11.3476   YZ=    -4.2293   ZZ=   157.1209
   Eigenvalues:   141.9329   153.9068   198.2554
 19  H    Isotropic =    29.8810   Anisotropy =    10.5541
   XX=    35.6116   YX=     2.8855   ZX=     2.4918
   XY=     1.9219   YY=    27.6992   ZY=     0.2369
   XZ=     2.6068   YZ=     0.7435   ZZ=    26.3324
   Eigenvalues:    25.6678    27.0582    36.9171
 20  H    Isotropic =    30.1703   Anisotropy =    10.8719
   XX=    34.1353   YX=    -4.9679   ZX=    -2.4064
   XY=    -4.3822   YY=    28.6824   ZY=     2.0268
   XZ=    -1.1507   YZ=     1.4424   ZZ=    27.6933
   Eigenvalues:    25.7314    27.3613    37.4183
 21  H    Isotropic =    30.0039   Anisotropy =     9.0690
   XX=    31.6980   YX=    -1.6965   ZX=     3.9970
   XY=    -0.9946   YY=    27.4639   ZY=    -3.5889
   XZ=     2.5255   YZ=    -3.8847   ZZ=    30.8500
   Eigenvalues:    24.9776    28.9843    36.0499

 ********************************************************************
Total atomic charges:
              1
  1  C   -0.329380
  2  C   -0.362005
  3  C   -0.288687
  4  H    0.181800
  5  H    0.179265
  6  C   -0.198573
  7  C   -0.335777
  8  C   -0.291550
  9  H    0.173572
 10  H    0.195105
 11  H    0.171676
 12  N   -0.188781
 13  H    0.195443
 14  H    0.174916
 15  H    0.224779
 16  H    0.197937
 17  H    0.208361
 18  C   -0.539609
 19  H    0.226989
 20  H    0.220618
 21  H    0.183900
 Sum of Mulliken charges=   0.00000
 Atomic charges with hydrogens summed into heavy atoms:
              1
  1  C    0.031685
  2  C    0.006673
  3  C   -0.117012
  4  H    0.000000
  5  H    0.000000
  6  C   -0.003130
  7  C    0.063919
  8  C    0.114748
  9  H    0.000000
 10  H    0.000000
 11  H    0.000000
```

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12  N   -0.188781
13  H    0.000000
14  H    0.000000
15  H    0.000000
16  H    0.000000
17  H    0.000000
18  C    0.091898
19  H    0.000000
20  H    0.000000
21  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=   848.9947
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=     0.5031    Y=     0.4340    Z=    -0.5601  Tot=     0.8690
Quadrupole moment (Debye-Ang):
  XX=   -50.2205   YY=   -50.6360   ZZ=   -51.6714
  XY=    -1.1386   XZ=     1.6608   YZ=     1.4700
Octapole moment (Debye-Ang**2):
 XXX=    -3.2312  YYY=    -2.6509  ZZZ=     0.0789  XYY=    -0.0960
 XXY=     1.8974  XXZ=    -1.1247  XZZ=     0.5181  YZZ=     1.4874
 YYZ=     1.2157  XYZ=    -1.6133
Hexadecapole moment (Debye-Ang**3):
XXXX=  -551.4489 YYYY=  -325.6186 ZZZZ=  -257.1859 XXXY=    -0.0094
XXXZ=     3.0932 YYYX=    -1.4175 YYYZ=     1.4207 ZZZX=     1.9783
ZZZY=     1.9089 XXYY=  -146.6063 XXZZ=  -143.7287 YYZZ=   -96.6937
XXYZ=     6.1152 YYXZ=     0.7095 ZZXY=    -3.1809
N-N= 4.144209428027D+02 E-N=-1.587892253760D+03  KE=
3.248954949049D+02
1|1|GINC-UNK|SP|RB3LYP|Gen|C7H13N1|PCUSER|12-Feb-1998|0||# HF/3-21G/B3
LYP EXTRABASIS NMR||endo 2-methyl-2-azabicyclo2.2.1heptane bdif//mm3||
0,1|C,0,0.,0.,0.|C,1,1.5578283763|C,1,1.5473672479,2,102.86985142|H,1,
1.1136721286,2,110.74425137,3,-118.32589248,0|H,1,1.1123088105,2,112.2
2174624,3,120.66225267,0|C,2,1.5443593785,1,103.23227754,3,0.71674027,
0|C,3,1.5370774509,1,100.88630366,2,-36.10167043,0|C,3,1.5449549832,1,
107.24945223,2,69.12117301,0|H,2,1.1134603226,1,110.35596631,3,118.604
90549,0|H,2,1.1105777505,1,112.41433806,3,-121.17893329,0|H,3,1.109876
1958,1,114.81320533,2,-161.71231565,0|N,6,1.4710687917,2,109.53670343,
1,-68.76983969,0|H,6,1.1087207313,2,115.97641578,1,161.4551201,0|H,7,1
.1119046047,3,113.08137674,1,-60.64056395,0|H,7,1.1125206066,3,112.870
97576,1,174.24515398,0|H,8,1.1191197121,3,111.86649984,1,46.14208824,0
|H,8,1.1153286063,3,111.71045988,1,168.50804886,0|C,12,1.4546910084,6,
118.06524764,2,-67.72047567,0|H,18,1.1113225499,12,110.12016587,6,-170
.62153569,0|H,18,1.1113488111,12,110.35960091,6,-51.66351178,0|H,18,1.
1228143658,12,111.62760462,6,69.23171737,0||Version=x86-Windows-G94Rev
D.3|HF=-327.8240374|RMSD=2.444e-009|Dipole=-0.3227822,0.0601764,-0.095
2893|PG=C01 [X(C7H13N1)]||@
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