Supporting information to the article "**Molecular Structure of 1,5-Diazabicyclo[3.1.0]hexane as Determined by Gas Electron Diffraction and Quantum-Chemical Calculations**".

Table S1. The most important geometrical parameters (Angstroms, degrees) of *cis*-N-methyl,N-ethyl-diaziridine (**A**, X=N) and *cis*-1-methyl,2-ethyl-cyclopropane (**B**, X=C) as calculated by MP2/6-31G(d) method [a].

Parameter	**A**	**B**
(X1-X5)	1.510	1.511
(X1-C6)	1.448	1.507
(X5-C6)	1.448	1.507
(X1-C2)	1.467	1.510
(X5-C4)	1.469	1.511
(C3-C4)	1.520	1.528
(X1-C6-X5)	62.8	60.2
(C6-X5-X1)	58.6	59.9
(X5-X1-C6)	58.6	59.9
(C6-X1-C2)	114.8	120.7
(C6-X5-C4)	115.5	121.4
(X5-X1-C2)	118.8	122.9
(X1-X5-C4)	118.8	122.7
(X5-C4-C3)	109.8	112.4
(X1-X5-C4-C3)	88.3	82.4
(C2-X1-X5-C4)	0.9	1.0

[a] See Figure 3 of the article for numeration.

Table S2. Calculated unscaled harmonic vibrational frequencies (cm^{-1}) and assignment of the DABH (boat conformer) as calculated by MP2/6-31G(d) and B3LYP/6-31G(df,p) methods.

Approximate description			MP2/6-31G(d)			B3LYP/6-31G(df,p)		
			wavenumber	I_{IR}[a]	A_{Ram}[b]	wavenumber	I_{IR}[a]	A_{Ram}[b]
A'	ν_1	CH_2 stretching	3268	16.2	76.4	3183	23.9	89.5
	ν_2	CH_2 stretching	3203	35.9	40.5	3126	49.1	54.9
	ν_3	CH_2 stretching	3178	6.2	59.3	3102	25.5	84.0
	ν_4	CH_2 stretching	3168	16.6	122.1	3097	13.8	135.8
	ν_5	CH_2 stretching	3143	10.5	65.4	3074	11.2	54.2
	ν_6	CH_2 stretching	3125	9.2	160.0	3062	17.1	176.7
	ν_7	CH_2 scissoring	1592	8.8	2.3	1541	5.5	2.6
	ν_8	CH_2 scissoring	1561	0.4	15.8	1509	0.1	16.6
	ν_9	CH_2 scissoring	1550	0.9	15.0	1497	1.2	17.4
	ν_{10}	CH_2 wagging	1402	0.9	4.5	1372	2.1	5.2
	ν_{11}	CN str. + CH def.	1309	12.7	8.3	1283	17.7	9.6
	ν_{12}	CH_2 twisting	1280	7.9	15.5	1252	4.8	18.1
	ν_{13}	CH_2 rocking	1212	0.9	0.9	1185	1.4	0.5
	ν_{14}	CH_2 rocking	1117	1.4	3.7	1090	1.8	3.4
	ν_{15}	ring mode	987	11.9	1.8	953	12.0	2.0
	ν_{16}	CC stretching	942	0.9	14.3	909	0.6	15.9
	ν_{17}	CN str. + CH_2 rocking	877	5.8	6.5	848	7.1	6.2
	ν_{18}	NN stretching	728	4.0	4.9	732	4.4	8.1
	ν_{19}	ring mode	644	0.6	3.0	638	0.6	3.4
	ν_{20}	ring flap	468	2.6	1.7	450	2.3	2.1
	ν_{21}	ring puckering	275	1.0	0.1	248	0.9	0.1
A"	ν_{22}	CH_2 stretching	3182	1.5	76.6	3102	4.8	90.3
	ν_{23}	CH_2 stretching	3123	43.9	8.0	3059	60.7	11.0
	ν_{24}	CH_2 scissoring	1552	1.6	10.1	1498	0.6	10.3
	ν_{25}	CH_2 def.	1381	0.0	4.8	1343	0.1	5.6
	ν_{26}	CH_2 wagging	1350	6.7	0.9	1318	3.5	0.6
	ν_{27}	CH_2 twisting	1242	8.0	0.7	1212	7.3	1.0
	ν_{28}	CH_2 twisting	1230	3.7	13.9	1200	4.6	14.7
	ν_{29}	CH_2 wagging	1189	4.5	0.4	1168	1.4	0.5
	ν_{30}	CH twist. + CN str.	1158	0.5	0.1	1132	1.1	0.4
	ν_{31}	CC str. + CH_2 twisting	1045	0.3	11.8	1008	1.7	11.0
	ν_{32}	ring mode	1003	9.2	3.3	977	10.8	3.1
	ν_{33}	CH_2 def.	923	0.0	0.8	893	0.0	1.2
	ν_{34}	CN stretching	770	10.3	4.8	745	10.3	4.9
	ν_{35}	ring def.	668	2.1	0.5	666	2.2	0.5
	ν_{36}	ring twisting	303	1.1	0.6	306	0.7	0.7

[a] IR intensities km mol^{-1}.

[b] Raman scattering activities $Å^4$ amu^{-1}.

Table S3. Experimental and theoretical mean square amplitudes and shrinkage corrections (in Angstroms) of the symmetry unique atomic pairs of the DABH molecule (boat conformer).

Term	$(r_a)_{exp}$	$\Delta(r_a\text{-}r_e)_{calc}$		$(l)_{calc}$		$(l)_{exp}$
		B3LYP/ 6-31G(df,p)	MP2/ 6-31G(d)	B3LYP/ 6-31G(df,p)	MP2/ 6-31G(d)	
C6-H7	1.1161	0.0162	0.0158	0.0762	0.0749	0.0749*
C6-H8	1.1200	0.0161	0.0160	0.0758	0.0753	0.0753*
C3-H12	1.1223	0.0161	0.0160	0.0764	0.0757	0.0757*
C3-H11	1.1226	0.0164	0.0159	0.0766	0.0756	0.0756*
C2-H13	1.1247	0.0164	0.0163	0.0767	0.0758	0.0758*
C2-H14	1.1254	0.0165	0.0162	0.0768	0.0759	0.0759*
N1-C6	1.4511	0.0084	0.0091	0.0492	0.0487	0.0494(13)[a]
N1-C2	1.4777	0.0084	0.0086	0.0516	0.0505	0.0512[a]
N1-N5	1.5157	0.0080	0.0095	0.0552	0.0558	0.0565[a]
C2-C3	1.5336	0.0097	0.0096	0.0525	0.0510	0.0517[a]
H11...H12	1.7778	0.0180	0.0179	0.1225	0.1206	0.1206*
H13...H14	1.8367	0.0187	0.0193	0.1226	0.1208	0.1208*
H7...H8	1.8858	0.0207	0.0204	0.1190	0.1174	0.1174*
N1...H13	2.0913	0.0159	0.0134	0.1057	0.1029	0.1029*
N1...H14	2.1239	0.0137	0.0154	0.1040	0.1046	0.1046*
N1...H7	2.1722	0.0166	0.0134	0.1011	0.1014	0.1014*
C3...H13	2.1981	0.0162	0.0169	0.1068	0.1049	0.1049*
C2...H11	2.2078	0.0163	0.0150	0.1070	0.1062	0.1062*
C2...H12	2.2082	0.0158	0.0166	0.1078	0.1053	0.1053*
N1...H8	2.2117	0.0137	0.0173	0.1024	0.1003	0.1003*
H7...H11	2.2179	0.0411	0.0378	0.2226	0.1217	0.1217*
C3...H14	2.2291	0.0173	0.0158	0.1066	0.1050	0.1050*
H11...H13	2.3762	0.0133	0.0130	0.1742	0.1700	0.1700*
N1...C3	2.4142	0.0142	0.0151	0.0581	0.0572	0.0595(25)[b]
C2...C4	2.4160	0.0144	0.0141	0.0622	0.0612	0.0635[b]
N1...C4	2.4165	0.0125	0.0132	0.0588	0.0587	0.0610[b]
H12...H14	2.4396	0.0146	0.0131	0.1730	0.1712	0.1712*
C2...C6	2.4684	0.0157	0.0155	0.0659	0.0653	0.0676[b]
C3...H7	2.5153	0.0339	0.0341	0.1532	0.1011	0.1011*
C2...H7	2.5877	0.0192	0.0218	0.1450	0.1009	0.1009*
H7...H13	2.6547	0.0066	0.0223	0.2282	0.1326	0.1326*
C3...C6	2.7634	0.0264	0.0258	0.0772	0.0732	0.0540(119)[c]
C6...H13	2.7985	0.0135	0.0211	0.1490	0.0997	0.0997*
H12...H13	2.8194	0.0231	0.0213	0.1532	0.1264	0.1264*
C6...H11	2.8953	0.0354	0.0315	0.1741	0.1000	0.1000*
N1...H11	2.9884	0.0241	0.0172	0.1349	0.1014	0.1014*
C2...H10	2.9940	0.0229	0.0177	0.1482	0.0990	0.0990*
N1...H10	3.0552	0.0183	0.0173	0.1348	0.1047	0.1047*
H11...H14	3.0994	0.0207	0.0223	0.1288	0.1513	0.1513*
H10...H14	3.1909	0.0257	0.0151	0.2458	0.1487	0.1487*
N1...H9	3.2410	0.0165	0.0182	0.1062	0.1339	0.0763(990)[d]
C2...H9	3.3244	0.0175	0.0219	0.1010	0.1448	0.0872[d]
N1...H12	3.3442	0.0163	0.0258	0.1036	0.1314	0.0738[d]
C6...H14	3.3946	0.0212	0.0130	0.1008	0.1471	0.0895[d]
C2...H8	3.4445	0.0223	0.0191	0.1022	0.1437	0.0861[d]

H7...H12	3.6153	0.0424	0.0481	0.1736	0.1849	0.1849*
H8...H13	3.6535	0.0209	0.0273	0.1771	0.1537	0.1537*
H7...H14	3.6689	0.0271	0.0200	0.1555	0.1752	0.1752*
C6...H12	3.8670	0.0315	0.0362	0.1026	0.1631	0.1631*
C3...H8	3.8749	0.0347	0.0333	0.1046	0.1469	0.1469*
H8...H11	3.9517	0.0474	0.0427	0.1967	0.1667	0.1667*
H10...H13	4.0401	0.0281	0.0277	0.1559	0.1538	0.1538*
H9...H13	4.0532	0.0139	0.0240	0.1543	0.2370	0.2370*
H8...H14	4.2818	0.0226	0.0065	0.1343	0.2255	0.2255*
H8...H12	4.9760	0.0377	0.0429	0.1240	0.2065	0.2065*

Total errors are given in parentheses.

[a], [b], [c],…[f] Grouped parameters in the least squares analysis.

* Fixed values.

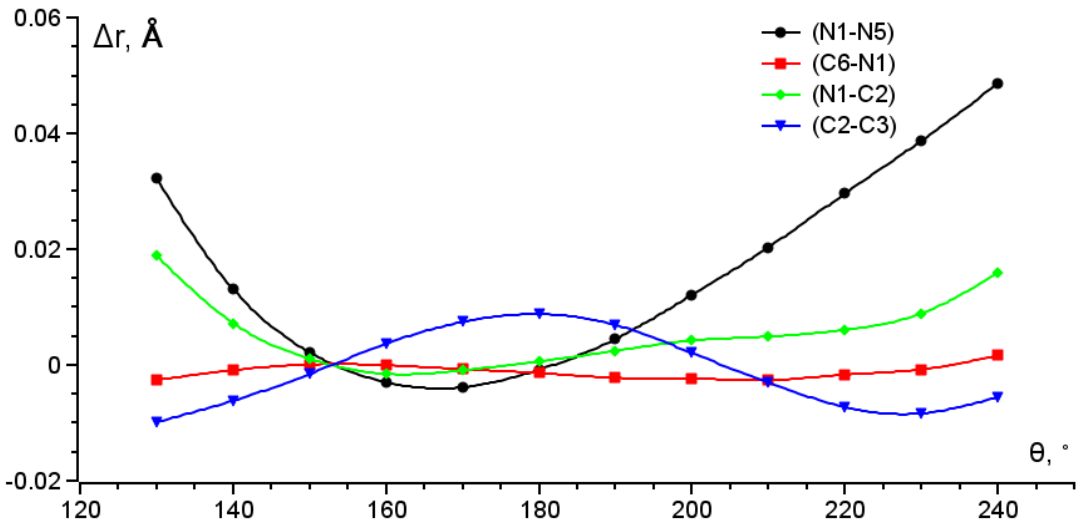

Figure S1. The differences between optimized bond lengths in a several DABH configurations with fixed angles θ and those for boat conformation with minimal energy. Δr=r(θ)-r(boat).

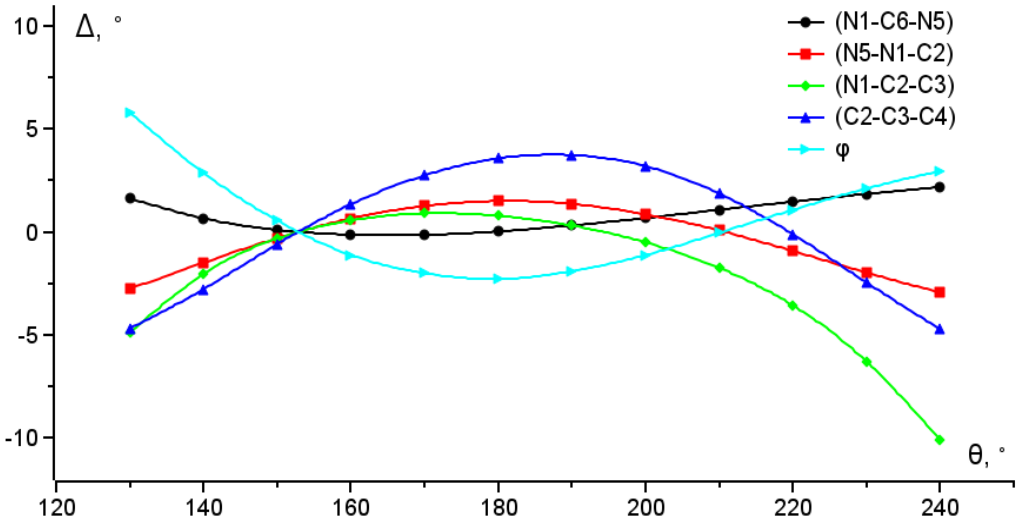

Figure S2. The differences between optimized angles in a several DABH configurations with fixed angles θ and those for boat conformation with minimal energy. Δ=∠(θ)-∠(boat).

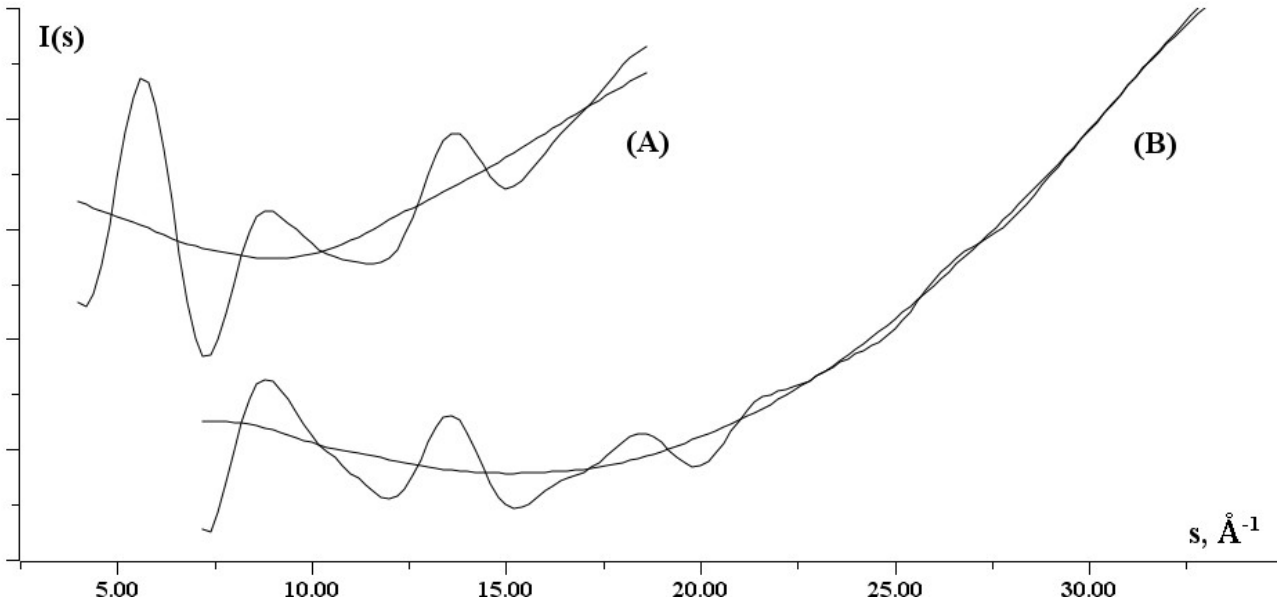

Figure S3. Intensities and the corresponding backgrounds for DABH as obtained from: (A) long camera distance, and (B) short camera distance.