Trimethylaluminum and borane complexes of primary amines

Balázs Németh[†‡], *Jean-Paul Guégan*[†], *Tamás Veszprémi*[*‡] *and Jean-Claude Guillemin*[*†]

[†]Sciences Chimiques de Rennes, Ecole Nationale Supérieure de Chimie de Rennes, CNRS, UMR 6226, Avenue du Général Leclerc, CS 50837, 35708 Rennes Cedex 7, France

[‡]Budapest University of Technology and Economics, Department of Inorganic and Analytical Chemistry, Budapest, Pf. 91, H-1521, Hungary

Received date: 26. 09. 2012.

*To whom correspondence should be addressed. E-mail: jean-claude.guillemin@ensc-rennes.fr (J.-C.G.), Tveszpremi@mail.bme.hu (T.V.).

Table of contents

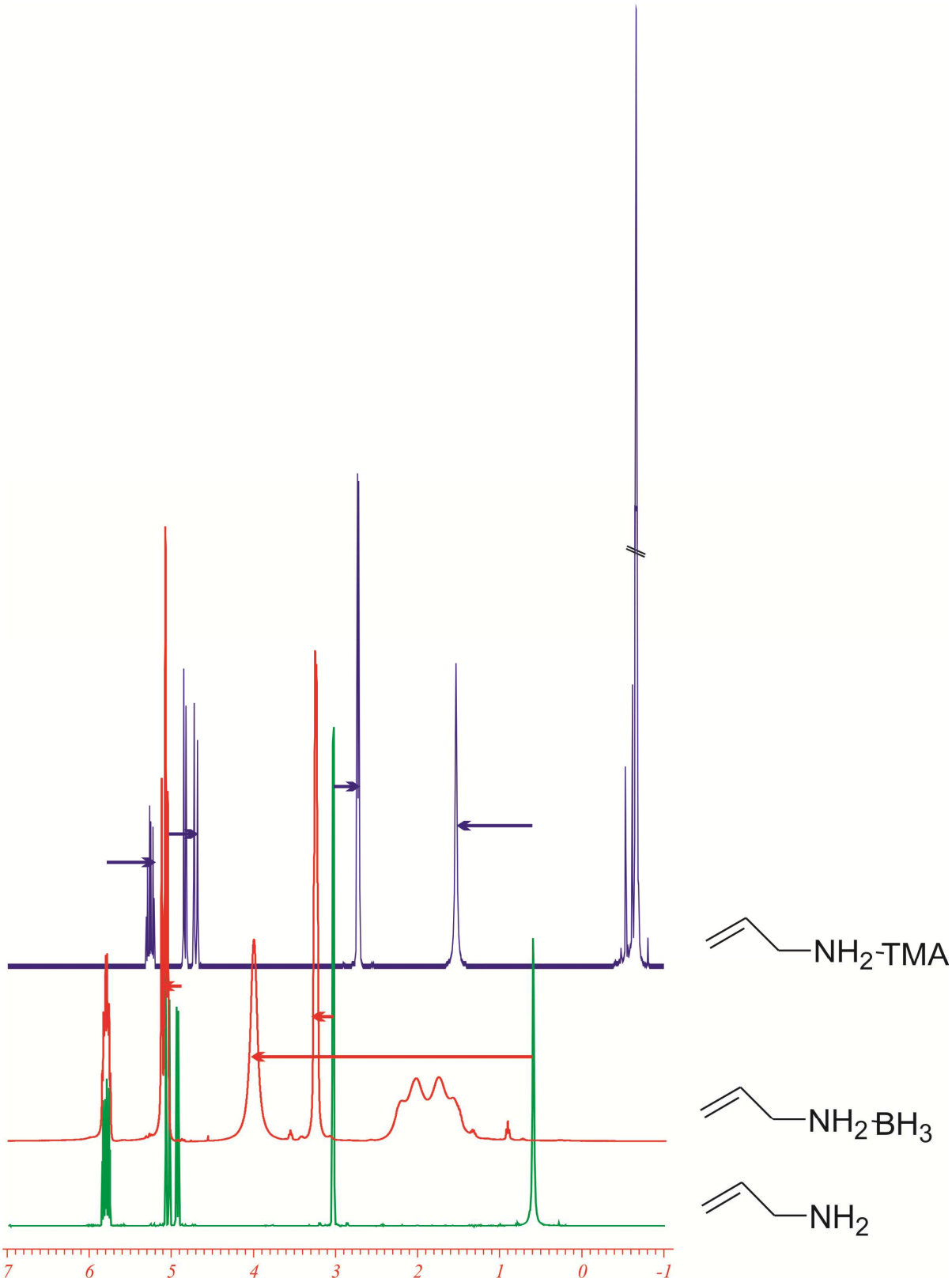

Figure S1. ^{1}H NMR chemical shift changes of allylamine with borane or trimethylaluminum complexation

(green/down: allylamine, red/middle: **4** blue/up: **9**, ***solv.: benzene***).

Figure S2. ^{27}Al, ^{13}C and ^{1}H NMR chemical shift changes of TMA upon allylamine addition (the indicated ratios are approximate values, solv.: benzene).

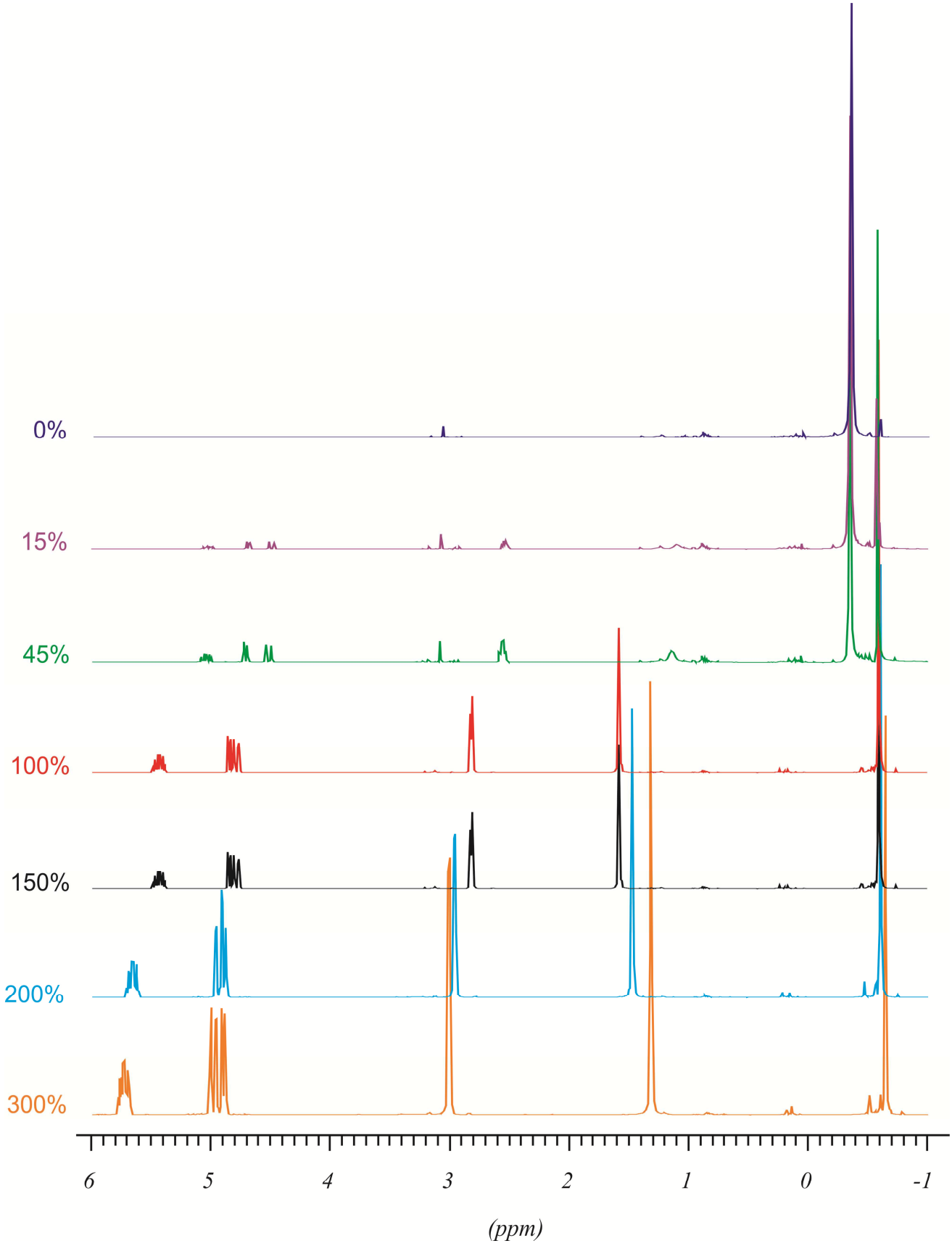

Figure S3. ^{1}H NMR chemical shift changes during allylamine addition to TMA (the indicated ratios are approximate values, solv.: benzene).

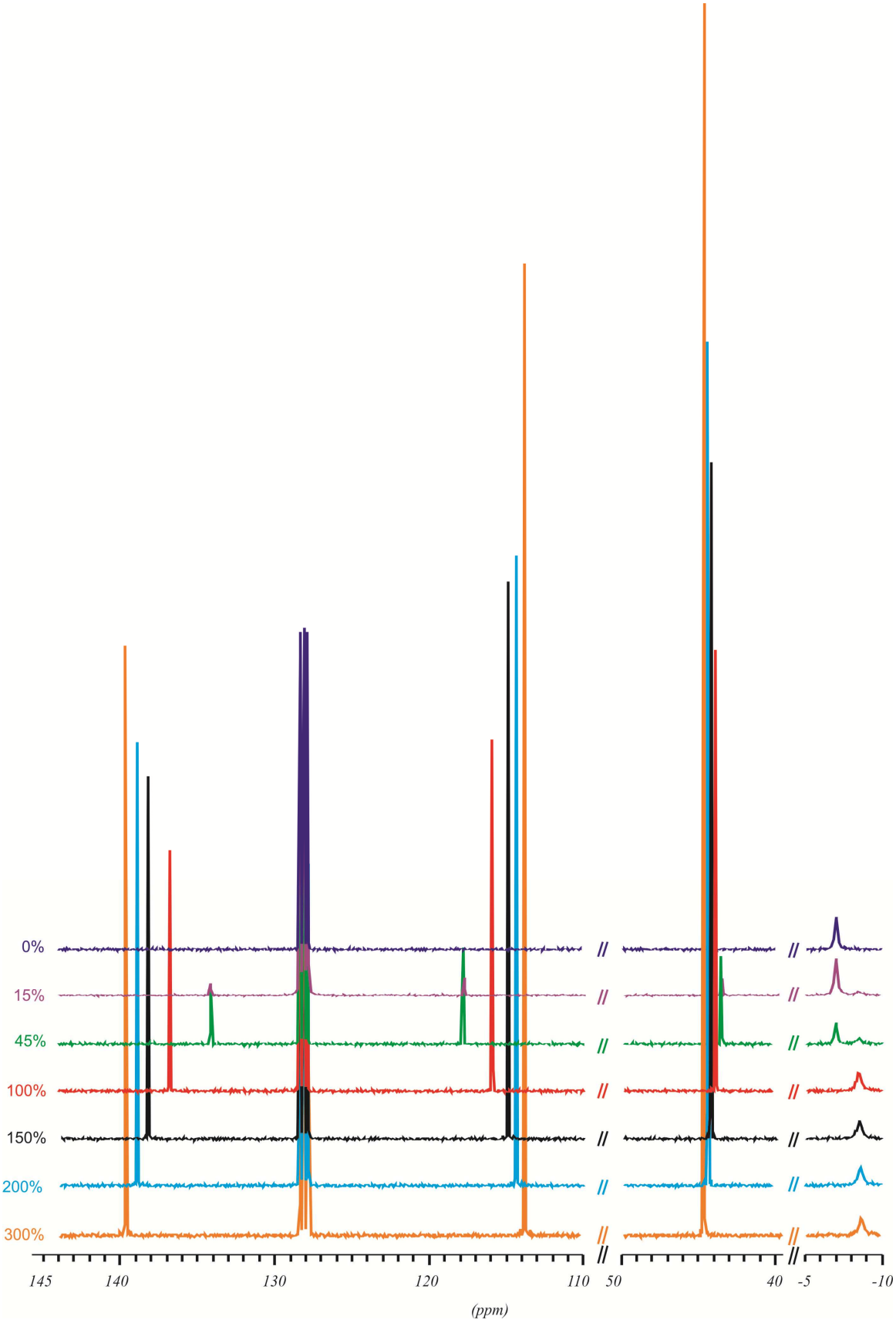

Figure S4. ^{13}C NMR chemical shift changes during allylamine addition to TMA

(the indicated ratios are approximate values, solv.: benzene, the triplet signal at 128 ppm belongs to it).

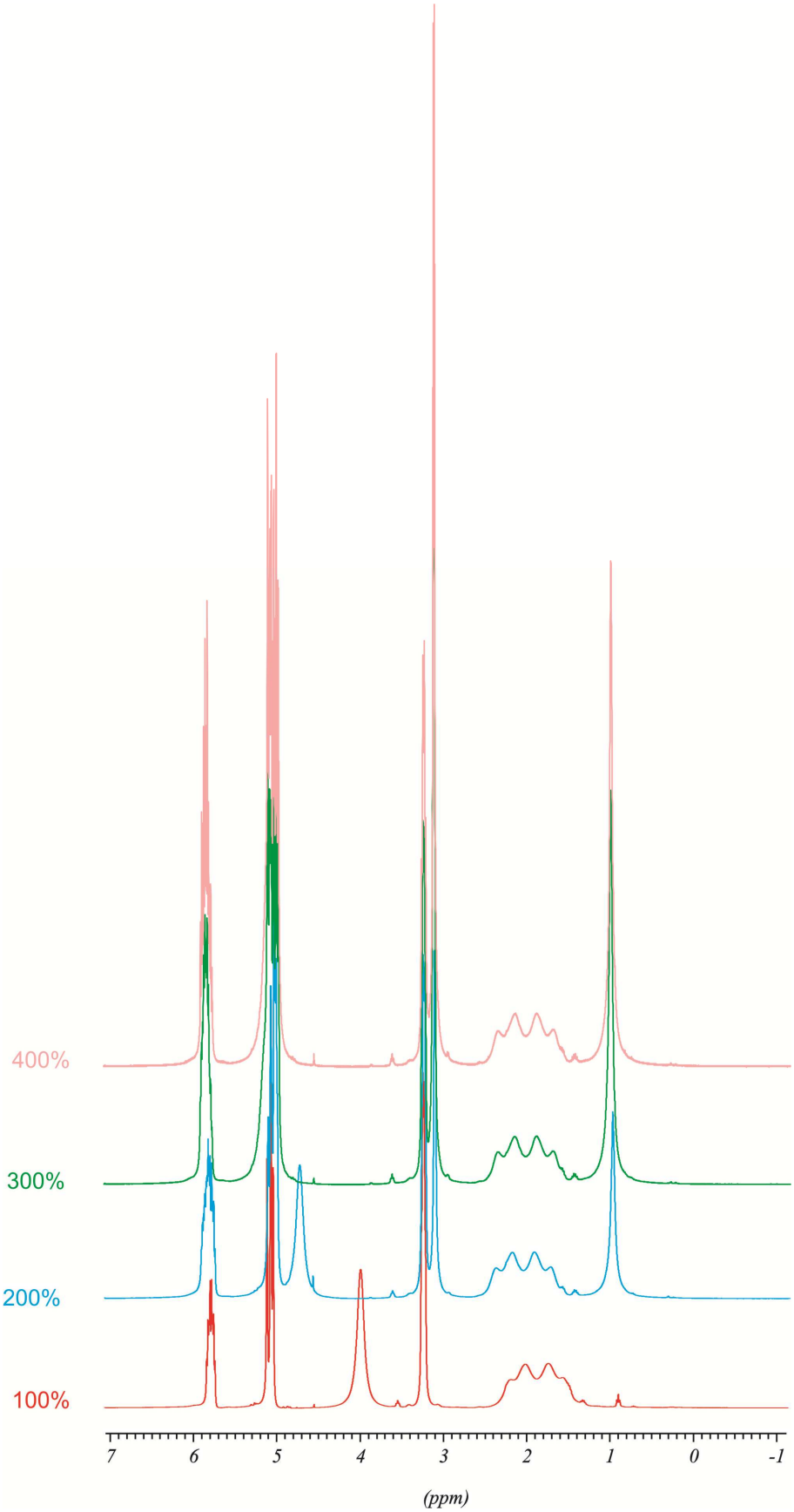

Figure S5. ^{1}H NMR chemical shift changes of allylamine-borane upon the addition of allylamine (the indicated ratios are approximate values, solv.: benzene).

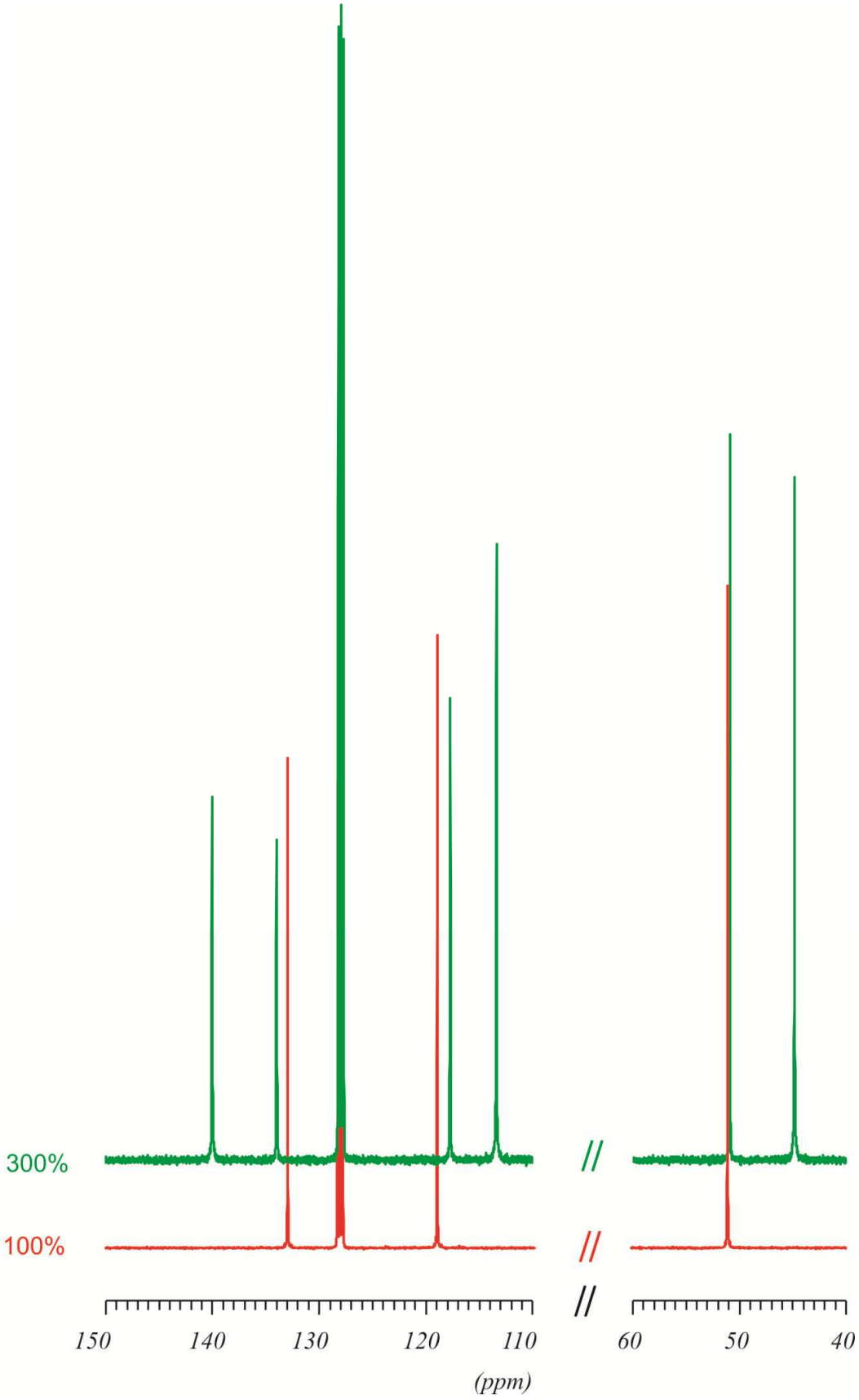

Figure S6. ^{13}C NMR chemical shift of the mixture of allylamine-borane and 2 equivalents of allylamine (the indicated ratios are approximate values, solv.: benzene).

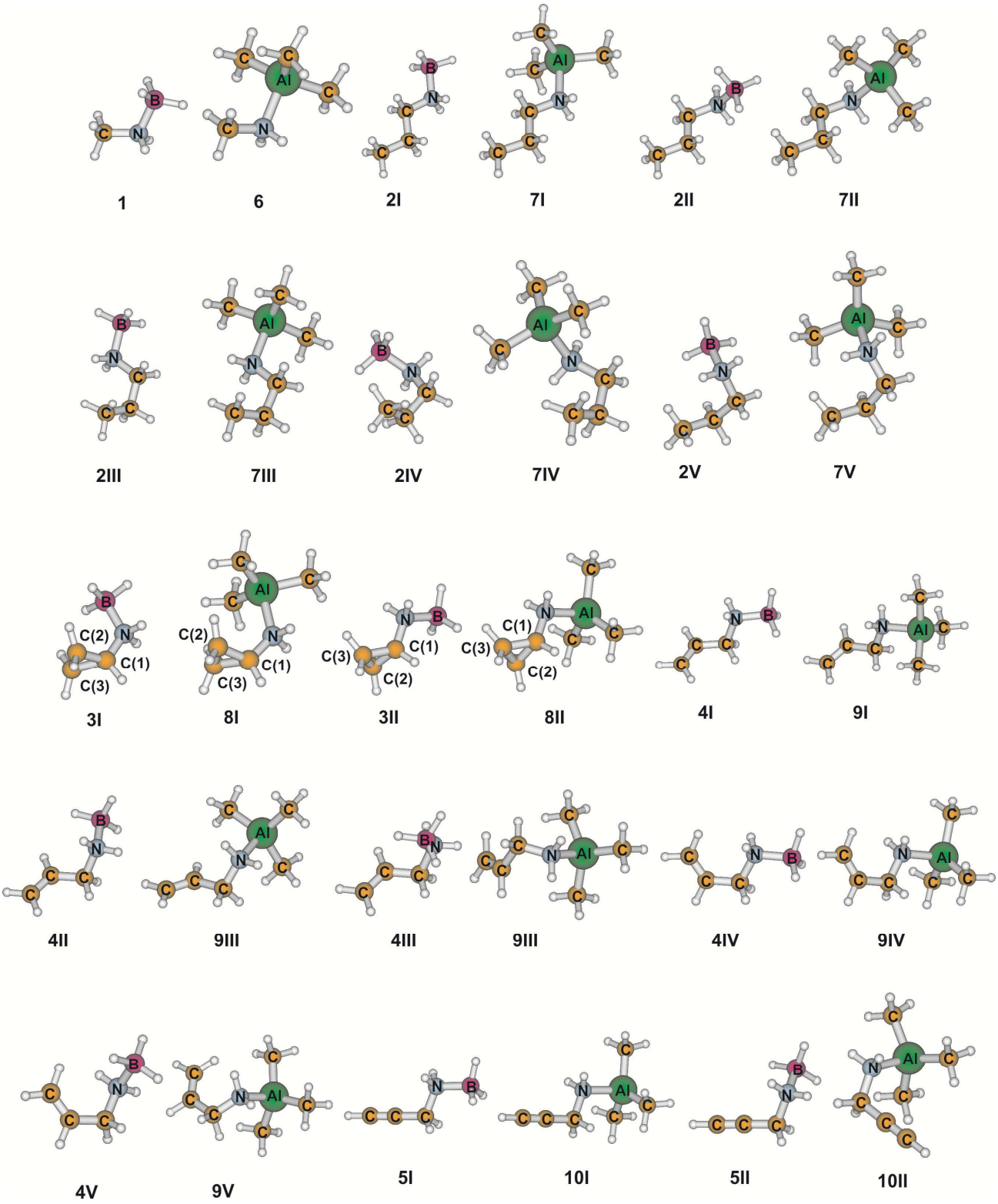

Figure S7. Optimized geometries of the obtained conformers of **1**-**10** (BMK/6-311++G(2df,p) level)

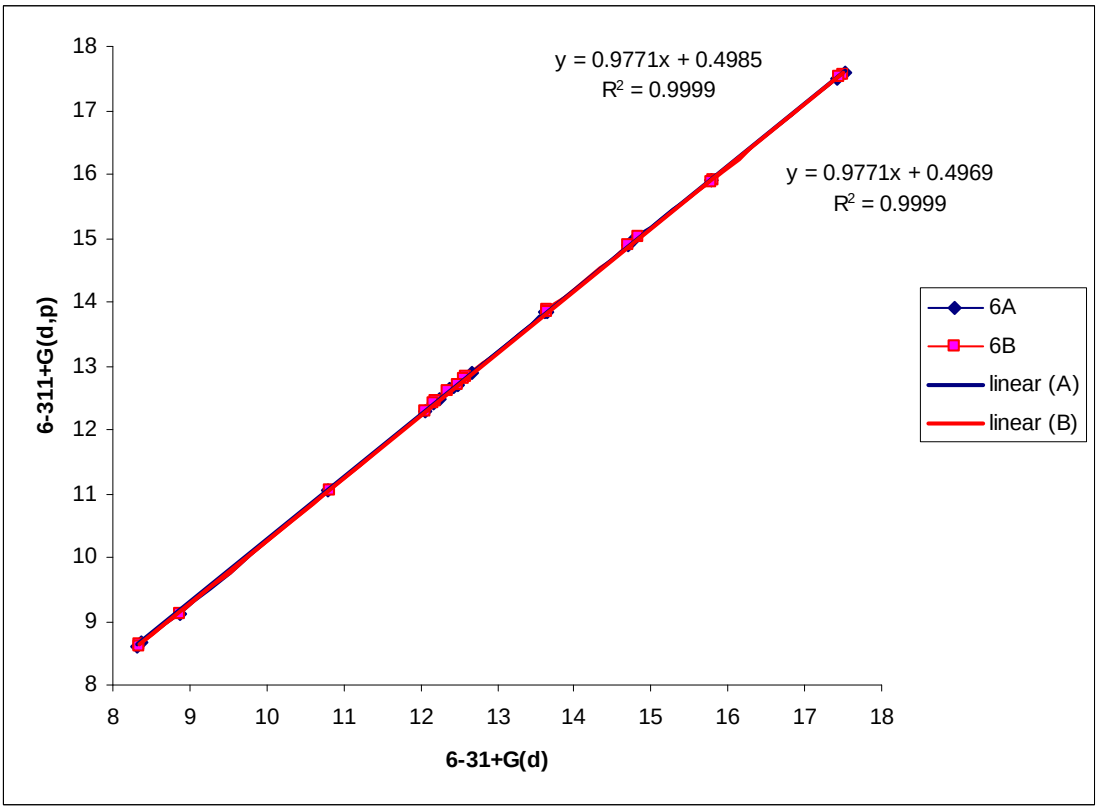

Figure S8. Correlation between OVGF/6-311+G(d,p) and OVGF/6-31+G(d) calculations in case of **6A** and **6B**.

Table S1. Relative energies of the studied amines and 1:1 complexes.[a]

No.		ΔE_{mes}[b]	ΔE_{calc}			ΔH_{calc} complexation	
-BH_3	-$AlMe_3$	amine	amine	-BH_3	-$AlMe_3$	-BH_3	-$AlMe_3$
1	**6**					-139.1	-93.7
2I	**7I**		0.0	0.0	0.0	-139.6	-94.5
2II	**7II**		0.3	6.0	4.9	-138.3	-93.6
2III	**7III**		0.9	2.5	1.9	-134.8	-90.9
2IV	**7IV**		1.0	15.9	13.6	-126.2	-82.4
2V	**7V**		1.6	7.6	4.9	-135.2	-92.3
3I	**8I**	o.	0.0	0.0	0.0	-126.3	-77.7
3II	**8II**	n. o.	6.6	-0.5	-5.1	-131.6	-88.8
4I	**9I**	0.18 ± 0.48	1.2	-0.1	1.1	-135.4	-89.8
4II	**9II**	n.o.	2.0	4.3	4.7	-131.8	-87.0
4III	**9III**	1.27 ± 0.18	8.0	10.0	9.9	-131.9	-88.3
4IV	**9IV**	0.0	0.0	0.0	0.0	-134.1	-89.2
4V	**9V**	o.[e]	1.4	11.3	8.5	-124.8	-82.8
5I	**10I**	o.	0.0	0.0	0.0	-130.7	-84.9
5II	**10II**	≥ 10.9	7.3	12.5	12.9	-125.3	-80.7

[a] Energy values are in kJ/mol, calculations performed at B3LYP/6-311+G(2df,p) + ZPE level.

[b] Microwave measurements (see Refs S1, S2, S3, S4). o. = observed, n. o.= not observed.

[c] V conformer of allylamine lies energetically higher than IV, but numerical determination was not possible (Ref. S3d).

Table S2. Calculated structural parameters of the investigated amines and their borane or trimethylaluminum complexes[a]

No.		N-B	N-Al	Al-C[b]		N-C		C(1)-C(2)/C(3)[c]			C(2)-C(3)			$\Sigma_{angle(N)}$[d]			$\Sigma_{angle(X)}$[e]	
-BH_3	-$AlMe_3$	-BH_3	-$AlMe_3$	-$AlMe_3$	amine	-BH_3	-$AlMe_3$	amine	-BH_3	-$AlMe_3$	amine	-BH_3	-$AlMe_3$	amine	-BH_3	-$AlMe_3$	-BH_3	-$AlMe_3$
1	**6**	1.616	2.064	1.974	1.461	1.475	1.476							329.0	326.1	326.5	339.2	350.8
2I	**7I**	1.615	2.066	1.975	1.459	1.478	1.478	1.537	1.529	1.531	1.534	1.534	1.534	328.6	322.9	325.7	338.0	350.5
2II	**7II**	1.619	2.075	1.975	1.461	1.484	1.481	1.530	1.527	1.528	1.533	1.534	1.533	329.1	325.3	325.3	339.4	349.7
2III	**7III**	1.615	2.063	1.975	1.459	1.479	1.479	1.540	1.531	1.533	1.534	1.535	1.535	328.8	325.2	326.0	338.9	350.3
2IV	**7IV**	1.616	2.090	1.976	1.463	1.486	1.488	1.534	1.539	1.530	1.533	1.535	1.533	328.9	324.3	324.5	338.5	348.6
2V	**7V**	1.617	2.072	1.975	1.463	1.485	1.483	1.532	1.529	1.530	1.535	1.535	1.535	327.8	325.4	325.0	338.9	349.4
3I	**8I**	1.625	2.094	1.975	1.438	1.469	1.460	1.527	1.513	1.526	1.519	1.528	1.516	331.0	323.5	323.8	338.4	348.5
3II	**8II**	1.620	2.072	1.973	1.438	1.459	1.457	1.533/1.510	1.504/1.518	1.533/1.508	1.529	1.533	1.519	330.5	324.0	326.3	338.2	350.8
4I	**9I**	1.615	2.068	1.974	1.464	1.483	1.482	1.511	1.505	1.506	1.329	1.327	1.327	328.5	324.8	325.3	339.0	350.9
4II	**9II**	1.619	2.077	1.975	1.463	1.489	1.485	1.506	1.504	1.504	1.328	1.328	1.327	328.6	324.4	324.9	338.6	349.9
4III	**9III**	1.618	2.078	1.974	1.466	1.488	1.485	1.506	1.503	1.505	1.327	1.325	1.326	328.1	324.5	325.1	339.1	350.4
4IV	**9IV**	1.617	2.067	1.975	1.452	1.470	1.470	1.516	1.506	1.508	1.328	1.328	1.327	329.8	325.7	326.0	339.2	350.8
4V	**9V**	1.622	2.092	1.976	1.456	1.480	1.476	1.508	1.506	1.504	1.328	1.326	1.327	329.1	324.4	324.8	339.1	349.6
5I	**10I**	1.616	2.073	1.974	1.461	1.480	1.479	1.477	1.466	1.467	1.198	1.196	1.196	327.0	324.8	324.9	339.5	351.3
5II	**10II**	1.620	2.095	1.973	1.464	1.487	1.483	1.468	1.462	1.463	1.197	1.195	1.195	328.5	325.0	325.5	339.7	351.2

[a] Calculated at BMK/6-311+G(2df,p) level of the theory, bond distances in Å, angles in degree.

[b] Average of the three Al-C bond lengths.

[c] In the cases of **3II** and **8II** C(1)-C(2) is different to C(1)-C(3) since their C_1 symmetry (see Figure S3).

[d] Sum of the bond angles around the N atom.

[e] Sum of the bond angles around the X atom (X=Al or B).

Table S3. Calculated NPA atomic charges of heavy atoms and hydrogen atoms on boron atom in the studied amines and 1:1 complexes at BMK/6-311+G(2df,p) level of the theory

No.		N			C(1)			C(2)			C(3)			B	Al	H[a]	C[b]	H[c]
-BH_3	-$AlMe_3$	amine	-BH_3	-$AlMe_3$	amine	-BH_3	-$AlMe_3$	amine	-BH_3	-$AlMe_3$	amine	-BH_3	-$AlMe_3$	-BH_3	-$AlMe_3$	-BH_3	-$AlMe_3$	-$AlMe_3$
1	**6**	-0.867	-0.696	-0.868	-0.366	-0.360	-0.373							-0.179	1.593	-0.062	-1.242	0.219
2I	**7I**	-0.862	-0.694	-0.868	-0.184	-0.178	-0.192	-0.410	-0.411	-0.407	-0.589	-0.584	-0.586	-0.180	1.594	-0.062	-1.241	0.218
2II	**7II**	-0.869	-0.696	-0.873	-0.180	-0.171	-0.191	-0.402	-0.416	-0.409	-0.586	-0.584	-0.595	-0.184	1.594	-0.062	-1.241	0.218
2III	**7III**	-0.866	-0.699	-0.873	-0.185	-0.177	-0.180	-0.410	-0.413	-0.415	-0.594	-0.595	-0.584	-0.179	1.595	-0.062	-1.243	0.218
2IV	**7IV**	-0.875	-0.695	-0.878	-0.180	-0.171	-0.179	-0.400	-0.414	-0.415	-0.591	-0.591	-0.601	-0.187	1.597	-0.061	-1.243	0.218
2V	**7V**	-0.874	-0.700	-0.884	-0.180	-0.169	-0.180	-0.401	-0.416	-0.405	-0.594	-0.602	-0.600	-0.188	1.604	-0.061	-1.246	0.219
3I	**8I**	-0.869	-0.692	-0.865	-0.052	-0.050	-0.053	-0.418	-0.418	-0.418	-0.418	-0.418	-0.418	-0.187	1.597	-0.060	-1.247	0.220
3II	**8II**	-0.857	-0.692	-0.862	-0.040	-0.037	-0.055	-0.420	-0.407	-0.412	-0.439	-0.427	-0.424	-0.178	1.598	-0.061	-1.242	0.218
4I	**a9I**	-0.854	-0.691	-0.864	-0.220	-0.212	-0.225	-0.201	-0.223	-0.216	-0.393	-0.354	-0.360	-0.180	1.594	-0.061	-1.241	0.219
4II	**a9II**	-0.866	-0.695	-0.864	-0.216	-0.206	-0.225	-0.187	-0.214	-0.216	-0.393	-0.363	-0.360	-0.183	1.594	-0.061	-1.241	0.219
4III	**a9III**	-0.861	-0.693	-0.870	-0.215	-0.205	-0.214	-0.183	-0.210	-0.217	-0.383	-0.345	-0.361	-0.184	1.595	-0.060	-1.243	0.219
4IV	**a9IV**	-0.858	-0.694	-0.866	-0.221	-0.215	-0.228	-0.193	-0.195	-0.193	-0.417	-0.402	-0.402	-0.177	1.595	-0.062	-1.242	0.219
4V	**a9V**	-0.867	-0.700	-0.875	-0.216	-0.208	-0.215	-0.193	-0.204	-0.202	-0.404	-0.385	-0.393	-0.182	1.603	-0.060	-1.248	0.220
5I	**a10I**	-0.841	-0.682	-0.852	-0.252	-0.244	-0.257	-0.045	-0.065	-0.060	-0.256	-0.206	-0.211	-0.181	1.591	-0.059	-1.243	0.220
5II	**a10II**	-0.850	-0.688	-0.858	-0.247	-0.238	-0.245	-0.026	-0.057	-0.060	-0.246	-0.195	-0.194	-0.182	1.599	-0.058	-1.246	0.220

[a] The average of the charge of the three hydrogen atoms in BH_3 moiety.

[b] The average of the charge of the three carbon atoms in TMA moiety.

[c] The average of the charge of the nine hydrogen atoms in TMA moiety.

The calculated NPA charges of the Lewis acid monomers at BMK/6-311+G(2df,p) level of the theory are: $\mathit{B}H_3$ 0.354, BH_3 0.118, $\mathit{Al}(CH_3)_3$ 1.744, $Al(\mathit{C}H_3)_3$ 1.280, $Al(C\mathit{H}_3)_3$ 0.233.

Table S4. Percentage participation in N-X (X=B, Al) dative bond and orbital coefficients according to NBO analysis at BMK/6-311+G(2df,p) level

	N				B					N				Al			
No.	s	p	d	f	s	p	d	f	**No.**	s	p	d	f	s	p	d	f
1		81.0				19.0			**6**		92.1				7.9		
	34.5	65.5	0.0	0.0	16.9	83.0	0.2	0.0		33.8	66.2	0.0	0.0	14.1	84.3	1.6	0.1
2I		80.9				19.1			**7I**		92.1				7.9		
	33.9	66.1	0.04	0	17	82.8	0.18	0.01		32.7	67.3	0.0	0.0	14.2	84.2	1.5	0.1
2II		80.8				19.2			**7II**		92.0				8.0		
	34.5	65.5	0.04	0	17	82.9	0.17	0.01		33.8	66.2	0.0	0.0	14.2	84.2	1.5	0.1
2III		80.9				19.1			**7III**		92.1				7.9		
	33.9	66.1	0.0	0.0	17.0	82.8	0.2	0.0		32.8	67.2	0.0	0.0	14.3	84.1	1.5	0.1
2IV		80.7				19.3			**7IV**		92.1				7.9		
	34.8	65.1	0.04	0	17	82.8	0.17	0.01		33.5	66.5	0.0	0.0	14.2	84.3	1.5	0.1
2V		80.7				19.3			**7V**		92.0				8.0		
	34.6	65.4	0.04	0	17.1	82.8	0.17	0.01		33.9	66.1	0.0	0.0	14.3	84.2	1.5	0.1
3I		80.8				19.2			**8I**		92.2				7.8		
	34.5	65.5	0.03	0	17	82.8	0.18	0.01		32.2	67.8	0.0	0.0	14.0	84.4	1.5	0.1
3II		81.1				18.9			**8II**		92.1				7.9		
	33.6	66.4	0.04	0	16.8	83	0.18	0.01		33.5	66.5	0.0	0.0	14.0	84.5	1.5	0.1
4I		80.9				19.1			**9I**		92.2				7.8		
	34	66	0.04	0	17	82.8	0.18	0.01		32.1	67.9	0.0	0.0	14.1	84.3	1.5	0.1
4II		80.9				19.1			**9II**		92.1				7.9		
	34.6	65.4	0.04	0	16.9	82.9	0.18	0.01		34.1	65.9	0.0	0.0	14.0	84.4	1.5	0.1
4III		81.0				19.0			**9III**		92.2				7.8		
	34.7	65.2	0.04	0	16.8	83	0.18	0.01		34.3	65.7	0.0	0.0	14.0	84.4	1.5	0.1
4IV		81.1				19.0			**9IV**		92.2				7.8		
	33.9	66.1	0.04	0	16.9	82.9	0.18	0.01		32.7	67.3	0.0	0.0	14.1	84.4	1.5	0.1
4V		81.0				19.0			**9V**		92.2				7.8		
	34.3	65.6	0.04	0	16.8	83	0.18	0.01		33.3	66.7	0.0	0.0	14.0	84.5	1.5	0.1
5I		81.0				19.0			**10I**		92.3				7.7		
	34	66	0.04	0	16.8	83	0.19	0.01		31.9	68.1	0.0	0.0	13.8	84.6	1.6	0.1
5II		81.2				18.8			**10II**		92.4				7.6		
	34.7	65.2	0.04	0	16.6	83.3	0.19	0.01		33.9	66.1	0.0	0.0	13.6	84.9	1.5	0.1

Table S5. Complexation enthalpies of the studied 1:1 complexes.[a]

No.		$R\text{-}NH_2 + LA \rightarrow RNH_2\text{-}LA$[b]		$2\ R\text{-}NH_2 + (LA)_2 \rightarrow 2\ RNH_2\text{-}LA$	
$-BH_3$	$-AlMe_3$	$-BH_3$	$-AlMe_3$	$-BH_3$	$-AlMe_3$
1	**6**	-139	-94	-120	-125
2I	**7I**	-140	-95	-95	-126
2II	**7II**	-135	-91	-105	-119
2III	**7III**	-138	-94	-121	-124
2IV	**7IV**	-126	-82	-112	-103
2V	**7V**	-135	-92	-119	-122
3I	**8I**	-126	-78	-113	-93
3II	**8II**	-132	-89	-95	-115
4I	**9I**	-135	-90	-113	-117
4II	**9II**	-132	-87	-105	-111
4III	**9III**	-132	-88	-106	-115
4IV	**9IV**	-134	-89	-110	-116
4V	**9V**	-125	-83	-92	-103
5I	**10I**	-131	-85	-103	-107
5II	**10II**	-125	-81	-92	-99

[a] Enthalpy values are in kJ/mol, calculations performed at BMK/6-311+G(2df,p) level. See Figure S7 for the different conformers.

[b] Counter Poise correction was used.[S5] LA= Lewis acid (BH_3 or $AlMe_3$).

Table S6. Calculated NPA atomic charges of heavy atoms and hydrogen atoms on boron atom in the studied amines and 2:1 complexes of amine-boranes at BMK/6-311+G(2df,p) level of the theory

	N^1	$C(1)^1$	$C(2)^1$	$C(3)^1$	N^2	$C(1)^2$	$C(2)^2$	$C(3)^2$	B/Al	H/C[a]
1A	-0.781	-0.365			-0.781	-0.365			-0.036	-0.094
1B	-0.781	-0.365			-0.781	-0.365			-0.037	-0.094
1H	-0.740	-0.359			-0.888	-0.381			-0.187	-0.066
2IAI	-0.778	-0.184	-0.405	-0.587	-0.778	-0.184	-0.405	-0.587	-0.032	-0.094
2IBI	-0.778	-0.183	-0.405	-0.587	-0.779	-0.183	-0.405	-0.587	-0.032	-0.094
2IHI	-0.740	-0.174	-0.410	-0.584	-0.892	-0.190	-0.408	-0.588	-0.192	-0.065
3IAI	-0.792	-0.048	-0.419	-0.418	-0.792	-0.048	-0.419	-0.418	0.006	-0.096
3IBI	-0.793	-0.047	-0.419	-0.419	-0.793	-0.047	-0.419	-0.419	0.010	-0.097
3IHI	-0.740	-0.046	-0.421	-0.419	-0.895	-0.048	-0.416	-0.420	-0.205	-0.060
3IAII	-0.785	-0.047	-0.420	-0.418	-0.785	-0.038	-0.414	-0.433	-0.008	-0.094
3IBII	-0.785	-0.047	-0.420	-0.419	-0.787	-0.038	-0.414	-0.433	-0.006	-0.094
3IHII	-0.737	-0.042	-0.422	-0.415	-0.887	-0.045	-0.425	-0.434	-0.203	-0.062
3IIHI	-0.739	-0.030	-0.409	-0.430	-0.882	-0.059	-0.417	-0.421	-0.191	-0.062
3IIAII	-0.779	-0.038	-0.413	-0.433	-0.779	-0.038	-0.413	-0.433	-0.020	-0.093
3IIBII	-0.779	-0.037	-0.414	-0.433	-0.780	-0.038	-0.414	-0.432	-0.018	-0.093
3IIHII	-0.734	-0.030	-0.411	-0.426	-0.890	-0.045	-0.426	-0.434	-0.193	-0.063
4IAI	-0.772	-0.219	-0.198	-0.386	-0.772	-0.219	-0.198	-0.386	-0.03	-0.093
4IBI	-0.772	-0.218	-0.199	-0.386	-0.772	-0.218	-0.199	-0.386	-0.031	-0.093
4IHI	-0.74	-0.208	-0.214	-0.364	-0.885	-0.225	-0.209	-0.375	-0.189	-0.064
4IAIV	-0.772	-0.219	-0.199	-0.386	-0.777	-0.222	-0.188	-0.414	-0.028	-0.093
4IBIV	-0.773	-0.219	-0.199	-0.386	-0.777	-0.221	-0.188	-0.414	-0.028	-0.093
4IHIV	-0.74	-0.209	-0.214	-0.363	-0.888	-0.227	-0.192	-0.41	-0.189	-0.064
4IVHI	-0.747	-0.211	-0.193	-0.402	-0.882	-0.226	-0.208	-0.375	-0.186	-0.065
4IVAIV	-0.777	-0.221	-0.188	-0.414	-0.777	-0.221	-0.188	-0.414	-0.026	-0.093
4IVBIV	-0.777	-0.221	-0.188	-0.414	-0.777	-0.221	-0.188	-0.414	-0.025	-0.093
4IVHIV	-0.748	-0.212	-0.193	-0.402	-0.881	-0.234	-0.188	-0.414	-0.186	-0.065
5IAI	-0.761	-0.251	-0.055	-0.233	-0.761	-0.252	-0.042	-0.248	-0.032	-0.091
5IBI	-0.761	-0.251	-0.042	-0.248	-0.761	-0.251	-0.042	-0.248	-0.029	-0.092
5IHI	-0.731	-0.246	-0.055	-0.219	-0.863	-0.267	-0.047	-0.239	-0.187	-0.063
5IAII	-0.763	-0.253	-0.040	-0.251	-0.772	-0.245	-0.029	-0.236	-0.027	-0.091
5IBII	-0.762	-0.251	-0.041	-0.249	-0.773	-0.245	-0.030	-0.236	-0.027	-0.091
5IHII	-0.729	-0.242	-0.052	-0.218	-0.872	-0.262	-0.035	-0.241	-0.189	-0.063
5IIHI	-0.731	-0.237	-0.048	-0.206	-0.875	-0.246	-0.052	-0.236	-0.190	-0.061
5IIAII	-0.776	-0.246	-0.027	-0.240	-0.775	-0.246	-0.027	-0.240	-0.024	-0.089
5IIBII	-0.776	-0.245	-0.028	-0.239	-0.776	-0.246	-0.028	-0.239	-0.022	-0.089
5IIHII	-0.735	-0.242	-0.043	-0.215	-0.872	-0.264	-0.039	-0.238	-0.190	-0.062
6A	-0.844	-0.373			-0.844	-0.373			1.539	-1.228
6B	-0.843	-0.371			-0.844	-0.372			1.535	-1.227
6H	-0.918	-0.371			-0.891	-0.364			1.598	-1.237
7IAI	-0.842	-0.193	-0.404	-0.586	-0.842	-0.193	-0.404	-0.586	1.542	-1.228
7IBI	-0.841	-0.191	-0.405	-0.586	-0.841	-0.193	-0.404	-0.586	1.539	-1.227
7IHI	-0.919	-0.188	-0.405	-0.586	-0.887	-0.191	-0.409	-0.588	1.600	-1.238
8IAI	-0.842	-0.423	-0.413	-0.049	-0.842	-0.422	-0.413	-0.048	1.569	-1.243
8IBI	-0.842	-0.422	-0.415	-0.048	-0.842	-0.415	-0.422	-0.049	1.562	-1.243
8IHI	-0.920	-0.046	-0.421	-0.414	-0.889	-0.051	-0.415	-0.418	1.607	-1.249
8IAII	-0.839	-0.415	-0.423	-0.048	-0.841	-0.050	-0.411	-0.428	1.555	-1.236
8IBII	-0.840	-0.414	-0.423	-0.048	-0.843	-0.049	-0.414	-0.424	1.552	-1.237
8IHII	-0.917	-0.045	-0.421	-0.415	-0.882	-0.045	-0.42	-0.432	1.606	-1.245
8IIHI	-0.911	-0.049	-0.414	-0.424	-0.890	-0.052	-0.415	-0.418	1.603	-1.240
8IIAII	-0.838	-0.048	-0.412	-0.427	-0.837	-0.048	-0.412	-0.429	1.545	-1.229
8IIBII	-0.837	-0.049	-0.413	-0.428	-0.837	-0.048	-0.415	-0.428	1.543	-1.230
8IIHII	-0.909	-0.048	-0.415	-0.424	-0.885	-0.431	-0.042	-0.420	1.606	-1.239

[a] The average of the charge of the three hydrogen/carbon atoms connected to boron/aluminum atom.

Table S6. Calculated NPA atomic charges of heavy atoms and hydrogen atoms on boron atom in the studied amines and 2:1 complexes of amine-boranes at BMK/6-311+G(2df,p) level of the theory (continued)

	N^1	$C(1)^1$	$C(2)^1$	$C(3)^1$	N^2	$C(1)^2$	$C(2)^2$	$C(3)^2$	B/Al	H/C[a]
9IAI	-0.838	-0.227	-0.205	-0.375	-0.837	-0.227	-0.204	-0.375	1.5394	-1.229
9IBI	-0.835	-0.225	-0.204	-0.376	-0.836	-0.226	-0.204	-0.375	1.5375	-1.227
9IHI	-0.912	-0.222	-0.209	-0.369	-0.883	-0.224	-0.212	-0.373	1.6008	-1.240
9IAIV	-0.838	-0.226	-0.205	-0.374	-0.839	-0.23	-0.188	-0.41	1.5405	-1.229
9IBIV	-0.835	-0.226	-0.205	-0.375	-0.84	-0.227	-0.189	-0.409	1.5394	-1.229
9IHIV	-0.912	-0.222	-0.209	-0.369	-0.885	-0.227	-0.195	-0.407	1.6001	-1.240
9IVHI	-0.919	-0.225	-0.19	-0.404	-0.88	-0.225	-0.211	-0.374	1.6028	-1.240
9IVAIV	-0.839	-0.230	-0.188	-0.410	-0.840	-0.229	-0.188	-0.410	1.545	-1.231
9IVBIV	-0.840	-0.229	-0.189	-0.409	-0.838	-0.227	-0.189	-0.409	1.542	-1.229
9IVHIV	-0.917	-0.226	-0.190	-0.404	-0.883	-0.226	-0.195	-0.407	1.602	-1.240
10IAI	-0.824	-0.258	-0.061	-0.219	-0.824	-0.257	-0.061	-0.219	1.539	-1.233
10IBI	-0.822	-0.257	-0.047	-0.235	-0.827	-0.258	-0.048	-0.232	1.534	-1.230
10IHI	-0.900	-0.256	-0.049	-0.226	-0.865	-0.258	-0.051	-0.237	1.598	-1.240
10IAII	-0.825	-0.259	-0.046	-0.235	-0.831	-0.250	-0.043	-0.218	1.540	-1.233
10IBII	-0.824	-0.258	-0.047	-0.235	-0.829	-0.248	-0.044	-0.216	1.543	-1.233
10IHII	-0.906	-0.255	-0.044	-0.229	-0.869	-0.262	-0.038	-0.241	1.599	-1.239
10IIHI	-0.903	-0.247	-0.052	-0.207	-0.867	-0.259	-0.052	-0.235	1.601	-1.241
10IIAII	-0.832	-0.251	-0.041	-0.223	-0.829	-0.249	-0.042	-0.219	1.546	-1.235
10IIBII	-0.837	-0.251	-0.042	-0.223	-0.830	-0.248	-0.040	-0.223	1.546	-1.235
10IIHII	-0.911	-0.246	-0.048	-0.211	-0.870	-0.263	-0.041	-0.240	1.602	-1.239

[a] The average of the charge of the three hydrogen/carbon atoms connected to boron/aluminum atom.

Table S7. Percentage participation in N-X (X=B, Al) dative bonds and orbital coefficients according to NBO analysis at BMK/6-311+G(2df,p) level in 2:1 complexes

	B/Al				N^1				B/Al				N^2			
No.	s	p	d	f	s	p	d	f	s	p	d	f	s	p	d	f
1A		5.6				94.4				5.6				94.4		
	22.1	53.9	23.7	0.4	24.1	75.9	0.1	0.0	22.1	53.9	23.7	0.4	24.1	75.8	0.1	0.0
1B		5.6				94.4				5.6				94.4		
	22.4	50.9	26.3	0.4	24.1	75.8	0.1	0.0	22.4	50.9	26.3	0.4	24.1	75.8	0.1	0.0
1H		19.7				80.3										
	17.5	82.4	0.2	0.0	33.3	66.6	0.1	0.0								
2IAI		5.5				94.5				5.5				94.5		
	21.0	52.4	26.2	0.4	22.7	77.2	0.1	0.0	21.0	52.4	26.2	0.4	22.7	77.2	0.1	0.0
2IBI		5.5				94.5				5.4				94.6		
	21.2	50.6	27.7	0.5	22.7	77.2	0.1	0.0	21.2	50.6	27.8	0.5	22.6	77.3	0.1	0.0
2IHI		19.9				80.1										
	17.7	82.1	0.2	0.0	32.8	67.2	0.1	0.0								
3IAI		4.6				95.4				4.7				95.3		
	19.2	51.8	28.7	0.3	22.5	77.4	0.1	0.0	19.3	51.8	28.7	0.3	22.5	77.4	0.1	0.0
3IBI		4.6				95.4				4.6				95.4		
	18.8	50.4	30.4	0.4	22.3	77.6	0.1	0.0	18.8	50.4	30.4	0.4	22.3	77.6	0.1	0.0
3IHI		19.9				80.1										
	17.6	82.2	0.2	0.0	33.4	66.6	0.0	0.0								
3IAII		5.2				94.8				4.6				95.4		
	20.2	51.5	28.0	0.3	23.2	76.7	0.1	0.0	19.8	51.1	28.8	0.4	20.7	79.2	0.1	0.0
3IBII		5.3				94.8				4.6				95.4		
	19.2	53.1	27.3	0.4	23.3	76.7	0.1	0.0	18.8	52.8	28.1	0.4	20.5	79.4	0.1	0.0

Table S7. Percentage participation in N-X (X=B, Al) dative bonds and orbital coefficients according to NBO analysis at BMK/6-311+G(2df,p) level in 2:1 complexes (continued)

	B/Al				N^1				B/Al				N^2			
No.	s	p	d	f	s	p	d	f	s	p	d	f	s	p	d	f
3IHII		20.0				80.0										
	17.7	82.1	0.2	0.0	33.5	66.5	0.0	0.0								
3IIHI		19.6				80.4										
	17.4	82.4	0.2	0.0	32.7	67.2	0.1	0.0								
3IIAII		5.2				94.8				5.2				94.8		
	20.4	52.6	26.7	0.4	21.4	78.5	0.1	0.0	20.4	52.6	26.7	0.4	21.4	78.5	0.1	0.0
3IIBII		5.2				94.8				5.1				94.9		
	20.7	50.7	28.1	0.5	21.4	78.6	0.1	0.0	20.8	50.6	28.2	0.5	21.2	78.7	0.1	0.0
4IAI		5.4				94.6				5.4				94.6		
	20.8	52.1	26.7	0.4	21.8	78.2	0.1	0.0	20.8	52.1	26.7	0.4	21.8	78.2	0.1	0.0
4IBI		5.4				94.6				5.4				94.6		
	21.0	50.4	28.1	0.5	21.9	78.1	0.1	0.0	21.0	50.4	28.1	0.5	21.9	78.1	0.1	0.0
4IHI		19.8				80.2										
	17.7	82.2	0.2	0.0	32.8	67.1	0.1	0.0								
4IAIV		5.4				94.6				5.4				94.6		
	20.7	52.7	26.2	0.4	21.8	78.2	0.1	0.0	20.7	52.7	26.2	0.4	22.5	77.5	0.1	0.0
4IBIV		5.4				94.6				5.4				94.6		
	21.0	50.4	28.1	0.5	21.8	78.2	0.1	0.0	20.9	50.6	28.0	0.5	22.5	77.4	0.1	0.0
4IHIV		19.8				80.2										
	17.6	82.2	0.2	0.0	32.7	67.2	0.1	0.0								
4IVHI		19.7				80.3										
	17.7	82.2	0.2	0.0	32.7	67.3	0.0	0.0								
4IVAIV		5.4				94.6				5.4				94.6		
	20.8	53.1	25.7	0.4	22.6	77.4	0.1	0.0	20.8	53.1	25.7	0.4	22.6	77.4	0.1	0.0
4IVBIV		5.3				94.7				5.3				94.7		
	21.0	50.6	27.9	0.5	22.4	77.5	0.1	0.0	21.0	50.6	27.9	0.5	22.5	77.5	0.1	0.0
4IVHIV		19.7				80.3										
	17.6	82.2	0.2	0.0	32.7	67.3	0.0	0.0								
5IAI		5.4				94.6				5.4				94.6		
	19.6	52.8	27.2	0.4	22.3	77.7	0.1	0.0	19.6	52.8	27.2	0.4	22.3	77.7	0.1	0.0
5IBI		5.3				94.7				5.3				94.7		
	19.5	50.6	29.4	0.5	22.1	77.9	0.1	0.0	19.5	50.6	29.4	0.5	22.1	77.8	0.1	0.0
5IHI		19.6				80.4										
	17.4	82.5	0.2	0.0	32.8	67.2	0.1	0.0								
5IAII		5.2				94.8				5.3				94.7		
	19.1	52.5	28.0	0.4	21.9	78.1	0.1	0.0	19.2	52.4	28.0	0.4	24.3	75.6	0.1	0.0
5IBII		5.3				94.8				5.2				94.8		
	19.2	51.6	28.7	0.5	21.8	78.1	0.1	0.0	19.3	51.4	28.8	0.5	24.2	75.7	0.1	0.0
5IHII		19.8				80.3										
	17.5	82.3	0.2	0.0	32.8	67.2	0.1	0.0								
5IIHI		19.5				80.6										
	17.2	82.7	0.2	0.0	33.6	66.3	0.0	0.0								
5IIAII		5.1				94.9				5.1				94.9		
	19.1	53.0	27.5	0.4	24.0	76.0	0.1	0.0	19.1	53.1	27.5	0.4	24.0	75.9	0.1	0.0
5IIBII		5.1				94.9				5.1				95.0		
	19.2	51.2	29.2	0.5	23.8	76.1	0.1	0.0	19.2	51.1	29.3	0.5	23.9	76.1	0.1	0.0
5IIHII		19.5				80.5										
	17.2	82.6	0.2	0.0	33.3	66.7	0.0	0.0								

Table S7. Percentage participation in N-X (X=B, Al) dative bonds and orbital coefficients according to NBO analysis at BMK/6-311+G(2df,p) level in 2:1 complexes (continued)

	B/Al				N^1				B/Al				N^2			
No.	s	p	d	f	s	p	d	f	s	p	d	f	s	p	d	f
6A		5.1				94.9				5.1				94.9		
	15.7	50.0	32.9	1.5	31.9	68.1	0.0	0.0	15.4	50.5	32.7	1.4	31.8	68.2	0.0	0.0
6B		5.1				94.9				5.1				94.9		
	15.5	50.2	32.7	1.6	31.5	68.5	0.0	0.0	15.7	49.8	32.9	1.6	31.9	68.1	0.0	0.0
6H		8.4				91.6										
	15.5	82.9	1.5	0.1	32.5	67.5	0.0	0.0								
7IAI		5.1				94.9				5.1				94.9		
	15.8	49.8	33.2	1.3	30.6	69.4	0.0	0.0	15.5	50.3	32.9	1.3	30.4	69.6	0.0	0.0
7IBI		5.1				94.9				5.1				94.9		
	15.7	50.1	32.9	1.4	30.2	69.8	0.0	0.0	15.8	49.9	33.0	1.4	30.4	69.6	0.0	0.0
7IHI		8.4				91.6										
	15.8	82.7	1.5	0.1	31.5	68.4	0.0	0.0								
8IAI		4.6				95.4				4.6				95.4		
	14.7	50.0	34.1	1.2	30.6	69.4	0.0	0.0	14.5	50.6	33.8	1.2	30.5	69.5	0.0	0.0
8IBI		4.7				95.3				4.6				95.4		
	14.7	50.4	33.9	1.1	30.5	69.5	0.0	0.0	14.9	49.9	34.2	1.1	30.5	69.4	0.0	0.0
8IHI		8.3				91.8										
	15.4	83.1	1.5	0.1	32.7	67.3	0.0	0.0								
8IAII		4.7				95.3				4.9				95.1		
	14.5	50.7	33.6	1.2	30.0	70.0	0.0	0.0	15.6	49.6	33.7	1.1	30.1	69.9	0.0	0.0
8IBII		4.8				95.2				4.8				95.2		
	14.8	50.6	33.3	1.3	30.4	69.6	0.0	0.0	15.4	50.0	33.4	1.3	29.1	70.9	0.0	0.0
8IHII		8.3				91.7										
	15.4	83.1	1.4	0.1	32.7	67.3	0.0	0.0								
8IIHI		8.2				91.8										
	15.3	83.2	1.5	0.1	31.0	69.0	0.0	0.0								
8IIAII		4.9				95.1				5.0				95.1		
	15.2	50.1	33.4	1.3	29.1	70.9	0.0	0.0	15.2	50.0	33.5	1.3	29.4	70.6	0.0	0.0
8IIBII		4.9				95.1				5.0				95.0		
	15.3	50.0	33.4	1.3	29.1	70.9	0.0	0.0	15.3	50.0	33.4	1.3	29.2	70.8	0.0	0.0
9IAI		5.1				94.9				5.1				94.9		
	15.8	49.8	33.2	1.3	29.7	70.3	0.0	0.0	15.5	50.4	32.9	1.3	29.4	70.6	0.0	0.0
9IBI		5.1				94.9				5.1				94.9		
	15.6	50.0	33.0	1.4	29.1	70.9	0.0	0.0	15.8	50.0	32.9	1.3	29.6	70.4	0.0	0.0
9IHI		8.3				91.7										
	15.4	83.1	1.5	0.1	30.7	69.3	0.0	0.0								
9IAIV		5.2				94.8				5.0				95.0		
	16.0	49.4	33.3	1.3	30.4	69.6	0.0	0.0	15.1	50.7	32.9	1.3	29.9	70.1	0.0	0.0
9IBIV		5.1				94.9				5.1				94.9		
	15.7	49.8	33.1	1.4	29.3	70.7	0.0	0.0	15.5	50.2	32.9	1.4	30.1	69.9	0.0	0.0
9IHIV		8.3				91.7										
	15.4	83.1	1.5	0.1	30.6	69.4	0.0	0.0								
9IVHI		8.3				91.8										
	15.5	83.0	1.5	0.1	31.3	68.7	0.0	0.0								
9IVAIV		5.0				95.0				5.0				95.0		
	15.6	49.8	33.4	1.2	30.4	69.6	0.0	0.0	15.4	50.3	33.1	1.2	30.2	69.8	0.0	0.0
9IVBIV		5.1				94.9				5.0				95.0		
	15.9	49.7	33.2	1.3	30.4	69.6	0.0	0.0	15.3	50.3	33.0	1.3	29.6	70.4	0.0	0.0
9IVHIV		8.2				91.8										
	15.4	83.1	1.5	0.1	31.0	69.0	0.0	0.0								

Table S7. Percentage participation in N-X (X=B, Al) dative bonds and orbital coefficients according to NBO analysis at BMK/6-311+G(2df,p) level in 2:1 complexes (continued)

	B/Al				N^1				B/Al				N^2			
No.	s	p	d	f	s	p	d	f	s	p	d	f	s	p	d	f
10IAI		5.0				95.0				5.0				95.0		
	15.3	49.8	33.7	1.2	29.2	70.8	0.0	0.0	15.1	50.3	33.4	1.2	29.0	71.0	0.0	0.0
10IBI		4.9				95.1				5.2				94.8		
	14.9	50.5	33.4	1.3	28.3	71.7	0.0	0.0	15.8	49.6	33.4	1.3	30.1	69.9	0.0	0.0
10IHI		8.2				91.8										
	15.0	83.4	1.5	0.1	30.4	69.6	0.0	0.0								
10IAII		5.0				95.0				4.9				95.1		
	15.4	50.2	33.2	1.2	29.1	70.9	0.0	0.0	15.3	50.0	33.5	1.3	31.8	68.2	0.0	0.0
10IBII		5.0				95.1				4.8				95.2		
	15.8	49.6	33.5	1.2	28.7	71.3	0.0	0.0	15.3	50.6	32.9	1.2	31.7	68.3	0.0	0.0
10IHII		8.3				91.7										
	15.1	83.3	1.5	0.1	30.7	69.3	0.0	0.0								
10IIHI		8.2				91.9										
	14.9	83.6	1.5	0.1	33.0	67.0	0.0	0.0								
10IIAII		4.8				95.2				4.8				95.2		
	15.7	49.6	33.5	1.3	31.5	68.5	0.0	0.0	15.4	50.5	32.9	1.3	31.7	68.3	0.0	0.0
10IIBII		4.8				95.2				4.8				95.2		
	15.7	49.8	33.3	1.3	31.0	68.9	0.0	0.0	15.5	50.4	32.8	1.3	31.2	68.8	0.0	0.0
10IIHII		8.2				91.8										
	15.1	83.3	1.5	0.1	33.3	66.7	0.0	0.0								

Evaluation of Ionization Energies

The Ionization Energies (IEs) were calculated for all conformers of 1:1 complexes, and some possible combination of the different amine conformers in case of 2:1 complexes (for the conformers see Figure S7 and Figure 2, the calculated IE values are in Table S8-14). From the calculated OVGF values, the weighted average of the estimated IEs (which can be found in the article, in Table 3) is calculated employing the Boltzmann distribution determined by the calculated relative energies of the conformers. The relative energies can be found in Table S5 and Table S15.

Table S8. Experimental and calculated Ionization Energies of **1**.[a]

calculated						measured	assign.
1:1			2:1				
	1A	**1B**	**1H**	pentacoord.	H-bonded		
est. distribution:				0	100		
10.57	8.62	8.61	9.94	8.61	9.94	10.29(3)	10a' σ_{B-H}
10.59	10.50	10.59	10.14	10.55	10.14	10.82(2)	3a" σ_{B-H}
12.40	10.72	10.64	10.47	10.68	10.47	12.47(2)	9a' σ_{N-B}
14.73	10.73	10.73	11.85	10.73	11.85	14.39(6)	2a" σ_{C-H}
15.00	13.41	13.41	13.72	13.41	13.72	14.90(9)	8a' σ_{C-H}
16.52	13.42	13.42	14.08	13.42	14.08	16.54(3)	7a' σ_{N-C}
18.20	14.03	14.02	14.57	14.02	14.57	17.83(2)	6a' σ_{B-H}
18.92	14.44	14.44	14.67	14.44	14.67	18.40(5)	1a" σ_{N-H}
	15.12	15.07	15.58	15.09	15.58		
	15.37	15.41	15.99	15.39	15.99		
	16.64	16.64	17.48	16.64	17.48		
	17.05	17.06	17.53	17.06	17.53		
	17.10	17.09	18.11	17.09	18.11		

[a] Calculations are performed by OVGF/6-311+G(d,p) method.

Table S9. Calculated Ionization Energies of **2**.[a]

calculated										
1:1						2:1				
	2I	**2II**	**2III**	**2IV**	**2V**	**2IAI**	**2IBI**	**2IHI**	pentacoord.	H-bonded
est. distribution:									0	100
10.42	10.42	10.39	10.41	10.38	10.40	8.40	8.40	9.76	8.40	9.76
10.46	10.46	10.48	10.46	10.49	10.48	10.05	10.07	10.00	10.06	10.00
11.92	11.89	12.02	11.96	11.91	11.95	10.65	10.64	10.15	10.64	10.15
12.94	12.96	12.72	12.98	12.56	12.62	10.65	10.65	11.46	10.65	11.46
13.10	13.14	12.86	13.08	12.70	12.86	12.06	12.06	12.22	12.06	12.22
13.74	13.89	13.13	13.57	12.90	13.05	12.07	12.07	12.47	12.07	12.47
14.31	14.21	14.33	14.55	14.30	14.75	12.24	12.23	12.54	12.24	12.54
15.02	14.85	14.92	15.52	15.05	15.04	12.35	12.35	12.79	12.35	12.79
16.10	16.31	16.06	15.63	15.48	15.39	12.93	12.89	13.29	12.91	13.29
16.53	16.52	16.58	16.56	16.60	16.55	13.25	13.25	13.36	13.25	13.36
17.72	17.64	17.93	17.85	18.14	18.02	13.25	13.25	13.59	13.25	13.59
18.76	18.82	18.40	18.71	18.25	18.57	13.26	13.28	13.82	13.27	13.82
						13.99	13.97	14.27	13.98	14.27
						14.19	14.19	14.50	14.19	14.50
						15.29	15.30	15.39	15.29	15.39
						15.31	15.32	15.40	15.32	15.40
						15.32	15.32	15.90	15.32	15.90
						15.33	15.33	16.02	15.33	16.02
						16.34	16.35	17.20	16.35	17.20
						17.15	17.16	17.24	17.15	17.24
						17.19	17.18	18.19	17.19	18.19

[a] Calculations are performed by OVGF/6-311+G(d,p) method.

Table S10. Experimental and calculated Ionization Energies of **3**.[a]

calculated														measured	assign.
1:1								2:1							
3I	**3II**	**3IAI**	**3IBI**	**3IHI**	**3IAII**	**3IBII**	**3IHII**	**3IIHI**	**3IIAII**	**3IIBII**	**3IIHII**	pentacoord.	H-bonded		
est. distribution:												0	100		
10.49	10.42	8.86	8.88	9.72	8.53	8.54	9.14	9.81	8.33	8.34	9.12	8.75	9.50	10.1	σ_{B-H}
10.55	10.48	9.91	9.92	10.28	9.73	9.75	10.21	9.99	9.42	9.42	10.17	9.83	10.19	10.8-11.2	σ_{B-H}
11.17	11.07	10.26	10.27	10.29	10.26	10.27	10.32	10.06	10.51	10.54	10.24	10.29	10.23		σ_{N-B}-σ_a
11.28	11.49	10.32	10.31	10.55	10.57	10.57	10.69	10.50	10.57	10.57	10.67	10.39	10.59	11.6	σ_s
12.43	13.13	10.68	10.69	10.82	10.86	10.83	10.80	10.60	10.72	10.75	10.69	10.72	10.74	13.1-13.6	σ_{N-B}+σ_a
13.62	13.95	11.07	11.08	10.90	10.88	10.90	10.94	11.08	10.77	10.82	11.14	11.01	11.02		σ_{C-H}
14.93	14.71	11.07	11.08	11.32	10.91	10.94	12.08	11.36	11.41	11.35	12.17	11.07	11.66	14.5	π_{ring}-σ_{C-N}
16.18	16.43	11.30	11.30	12.13	11.98	11.96	12.24	12.73	12.26	12.25	12.83	11.53	12.49	16.1	σ_{ring}
17.06	17.31	12.93	12.96	13.24	12.94	12.96	13.23	12.96	13.15	13.16	13.21	12.96	13.18	16.9	π_{ring}+σ_{C-N}
18.25	17.79	13.00	13.01	13.35	13.16	13.17	13.33	13.64	13.16	13.17	13.65	13.05	13.51		
18.25	18.74	13.86	13.89	14.11	13.55	13.55	13.72	14.07	13.54	13.53	13.70	13.77	13.94		
		13.89	13.89	14.59	13.87	13.88	14.57	14.30	13.55	13.56	14.32	13.86	14.44		
		15.40	15.39	15.66	15.39	15.41	15.62	15.58	15.50	15.52	15.56	15.41	15.61		
		15.45	15.49	15.88	15.60	15.62	15.82	15.99	15.66	15.71	16.01	15.51	15.94		
		16.34	16.34	16.50	16.14	16.15	16.14	16.85	16.14	16.15	16.27	16.28	16.47		
		16.47	16.48	16.76	16.36	16.36	16.69	16.88	16.15	16.16	16.88	16.42	16.82		
		16.52	16.51	17.16	16.48	16.49	17.30	17.12	16.40	16.37	17.22	16.50	17.18		
		16.93	16.97	17.67	17.00	17.00	17.64	17.18	17.17	17.17	17.30	16.98	17.45		
		17.06	17.05	17.81	17.21	17.20	17.81	18.11	17.25	17.23	18.25	17.10	18.02		

[a] Calculations are performed by OVGF/6-311+G(d,p) method.

Table S11. Experimental and calculated Ionization Energies of **4**.[a]

calculated															measurec	assign.
4I	**4II**	**4III**	**4IV**	**4V**	**4IAI**	**4IBI**	**4IHI**	**4IAIV**	**4IBIV**	**4IHIV**	**4IVHI**	**4IVAIV**	**4IVBIV**	**4IVHIV**	measured	assign.
10.52	10.48	10.21	10.55	10.19	8.78	8.77	9.76	8.93	8.94	9.93	9.74	8.71	8.72	9.92	10.1	σ_{B-H}
10.63	10.54	10.43	10.58	10.51	9.81	9.80	10.22	9.65	9.62	10.12	10.15	9.85	9.85	10.08	10.7	π
10.65	10.56	10.60	10.70	10.70	9.90	9.90	10.24	9.84	9.84	10.21	10.26	9.87	9.85	10.24		σ_{B-H}
12.21	12.19	12.30	12.23	12.34	10.46	10.59	10.27	10.44	10.62	10.29	10.28	10.42	10.62	10.25	12.2-12.5	σ_{N-B}
13.53	13.07	12.99	13.69	13.09	10.77	10.66	10.31	10.80	10.64	10.33	10.30	10.83	10.63	10.30	13.3	σ_{C-H}
14.18	14.35	14.17	14.46	14.35	10.78	10.77	11.82	10.81	10.81	11.83	11.82	10.85	10.85	11.80	14.1	σ_{C-H}
15.21	15.09	14.96	14.87	15.03	12.60	12.58	12.80	12.66	12.64	12.94	12.80	12.75	12.72	12.96	15.0	σ_{C-C}
15.75	15.64	15.98	16.21	15.71	12.83	12.83	13.18	12.90	12.92	13.22	13.30	12.95	12.96	13.33		
16.84	16.79	16.67	16.59	16.61	13.11	13.10	13.33	13.14	13.11	13.67	13.34	13.44	13.44	13.65		
17.73	17.86	18.09	18.15	18.11	13.18	13.18	13.81	13.52	13.51	13.77	14.04	13.60	13.61	13.83		
18.78	18.51	18.11	18.88	18.74	14.47	14.47	14.68	13.67	13.67	13.87	14.37	13.68	13.68	14.03		
					14.59	14.60	14.87	14.57	14.55	14.96	14.67	13.69	13.68	14.41		
					14.67	14.67	14.91	14.75	14.75	15.30	14.83	15.30	15.28	15.40		
					14.87	14.87	15.28	15.30	15.30	15.39	15.80	15.30	15.32	15.82		
					15.79	15.78	15.85	15.76	15.75	16.05	15.88	15.62	15.61	16.01		
					15.80	15.82	16.41	15.83	15.84	16.44	16.11	16.02	16.02	16.17		
					16.50	16.50	17.22	16.67	16.67	17.23	17.21	16.77	16.80	17.27		
					17.18	17.19	17.30	17.17	17.18	17.31	17.70	17.17	17.18	17.68		
					17.22	17.21	18.24	17.22	17.21	18.28	18.24	17.22	17.19	18.27		
					18.87	18.88	18.94	18.59	18.59	18.68	18.92	18.60	18.60	18.69		
					18.90	18.89		18.90	18.89			18.61	18.60			

[a] Calculations are performed by OVGF/6-311+G(d,p) method.

Table S12. Experimental and calculated Ionization Energies of **5**.[a]

calculated												measured	assign.
5I	**5II**	**5IAI**	**5IBI**	**5IHI**	**5IAII**	**5IBII**	**5IHII**	**5IIHI**	**5IIAII**	**5IIBII**	**5IIHII**		
10.67	10.43	9.06	9.08	10.29	9.05	9.05	10.13	10.20	9.04	9.05	9.95	10.4	$\sigma_{B\text{-}H}$
10.68	10.59	10.39	10.39	10.40	10.22	10.21	10.46	10.28	10.08	10.10	10.18		$\sigma_{B\text{-}H}$
11.21	11.01	10.42	10.40	10.44	10.33	10.36	10.48	10.41	10.25	10.23	10.41	11.2-11.6	π_1
11.35	11.06	10.47	10.46	10.44	10.36	10.38	10.60	10.59	10.37	10.37	10.52		π_2
12.77	12.58	10.54	10.53	10.93	10.52	10.51	10.66	10.73	10.48	10.48	10.76	12.7	$\sigma_{N\text{-}B}$
15.23	15.37	11.04	11.05	10.96	10.94	10.92	10.68	10.79	10.87	10.83	10.86	14.9-15.1	$\sigma_{C\text{-}H,}$ $\sigma_{C\text{-}N\text{-}H}$
15.68	15.61	11.04	11.05	11.05	10.98	10.99	10.92	10.91	10.87	10.90	10.96	15.4-15.7	$\sigma_{N\text{-}C}$
16.87	16.84	11.16	11.15	12.38	11.00	11.03	12.34	12.24	10.89	10.92	12.06		
18.08	18.16	14.18	14.17	14.45	14.09	14.13	14.51	14.42	14.36	14.36	14.77		
19.09	18.36	14.19	14.18	14.92	14.43	14.42	14.78	15.05	14.36	14.38	14.87		
		14.90	14.89	15.18	14.82	14.82	15.19	15.19	14.72	14.72	15.00		
		15.06	15.06	15.30	15.02	15.03	15.24	15.32	15.11	15.00	15.46		
		15.78	15.73	16.25	15.74	15.70	16.11	16.30	15.64	15.61	16.17		
		16.13	16.15	16.44	16.03	16.08	16.44	16.48	15.99	16.04	16.45		
		16.96	16.96	17.68	16.88	16.88	17.40	17.54	16.80	16.80	17.62		
		17.47	17.47	17.72	17.27	17.24	17.65	17.75	17.16	17.15	17.65		
		17.52	17.50	18.11	17.37	17.41	18.20	18.00	17.21	17.22	17.75		
		18.01	18.01	18.57	17.97	18.00	18.41	18.17	18.03	18.02	18.45		
		18.06	18.05	18.70	18.08	18.07	18.63	18.80	18.03	18.05	18.61		

[a] Calculations are performed by OVGF/6-311+G(d,p) method.

Table S13. Experimental and calculated Ionization Energies of **6-9**.[a]

calculated															measured	assign.
6	**6A**	**6B**	**6H**													
8.96	8.63	8.64	8.80												9.0	2 σ_{Al-C}
8.96	8.67	8.65	8.82													
10.83	9.16	9.15	10.19												10.7	σ_{N-Al}
	11.06	11.07	10.63													
7I	**7II**	**7III**	**7IV**	**7V**	**7IAI**	**7IBI**	**7IHI**									
8.88	8.88	8.87	8.87	8.89	8.55	8.56	8.74								8.8-9.0	2 σ_{Al-C}
8.89	8.91	8.88	8.92	8.90	8.60	8.59	8.74									
10.63	10.70	10.65	10.73	10.68	8.98	8.98	9.83								10.6	σ_{N-Al}
					10.60	10.60	10.38									
8I	**8II**	**8IAI**	**8IBI**	**8IHI**	**8IAII**	**8IBII**	**8IHII**	**8IIHI**	**8IIAII**	**8IIBII**	**8IIHII**					
8.98	8.89	8.75	8.75	8.83	8.66	8.64	8.81	8.75	8.55	8.58	8.76				8.9-9.1	2 σ_{Al-C}
8.99	8.90	8.78	8.79	8.85	8.70	8.69	8.82	8.80	8.62	8.59	8.81					
10.75	10.35	9.28	9.29	9.94	9.09	9.12	9.43	9.83	8.91	8.90	9.40				10.4	σ_{N-Al} (σ_{cyc})
11.21	11.41	10.26	10.29	10.42	10.13	10.16	10.37	10.18	9.92	9.92	10.05				11.4	2 σ_{cyc}
11.33	11.65	10.64	10.63	10.73	10.56	10.59	10.92	10.73	10.79	10.79	10.98					
		10.65	10.65	10.94	10.87	10.81	10.93	11.07	10.83	10.83	11.07					
		10.80	10.80	11.10	10.81	10.84	11.08	11.42	11.01	11.00	11.41					
		11.35	11.35	11.45	11.70	11.71	12.45	11.45	12.02	12.02	12.43					
9I	**9II**	**9III**	**9IV**	**9V**	**9IAI**	**9IBI**	**9IHI**	**9IAIV**	**9IBIV**	**9IHIV**	**9IVHI**	**9IVAIV**	**9IVBIV**	**9IVHIV**		
8.93	8.93	8.83	8.95	8.91	8.64	8.64	8.81	8.66	8.66	8.82	8.80	8.68	8.69	8.82	9.0-9.2	2 σ_{Al-C}
8.93	8.95	8.88	8.95	8.93	8.67	8.66	8.81	8.68	8.68	8.82	8.82	8.71	8.70	8.84		
10.62	10.57	10.36	10.66	10.35	9.30	9.32	9.93	9.42	9.45	10.15	9.93	9.21	9.22	10.16	10.5	π
10.91	10.78	10.83	10.80	10.85	10.07	10.07	10.30	9.97	9.92	10.16	10.28	10.17	10.16	10.17	11.0	σ_{N-Al}
					10.21	10.22	10.30	10.14	10.17	10.31	10.37	10.18	10.19	10.36		
					11.03	11.01	10.70	11.01	11.00	10.69	10.60	10.97	10.97	10.58		

[a] Calculations are performed by OVGF/6-311+G(d,p) method for 1:1 adducts and scaled OVGF/6-31+G(d) method for 2:1 adducts.

Table S14. Experimental and calculated Ionization Energies of **10**.[a]

calculated												measured	assign.
10I	**10II**	**10IAI**	**10IBI**	**10IHI**	**10IAII**	**10IBII**	**10IHII**	**10IIHI**	**10IIAII**	**10IIBII**	**10IIHII**		
9.04	8.90	8.82	8.81	8.90	8.69	8.67	8.76	8.76	8.64	8.61	8.66	9.0-9.2	2 σ_{Al-C}
9.04	8.94	8.85	8.84	8.93	8.78	8.77	8.78	8.84	8.65	8.67	8.76		
10.88	10.82	9.48	9.46	10.48	9.45	9.48	10.52	10.52	9.46	9.43	10.43	10.7	σ_{N-Al}-π_1
11.15	11.03	10.73	10.72	10.74	10.37	10.37	10.64	10.71	10.44	10.42	10.63	11.1	π_2
11.33	11.07	10.75	10.77	10.75	10.69	10.68	10.83	10.73	10.42	10.46	10.73	11.6	σ_{N-Al}+π_1
		10.78	10.78	10.92	10.71	10.70	10.84	10.74	10.55	10.63	10.74		
		10.85	10.86	10.96	10.74	10.70	10.94	10.94	10.62	10.69	11.13		
		11.67	11.69	11.20	11.53	11.49	11.05	11.21	11.36	11.38	11.00		

[a] Calculations are performed by OVGF/6-311+G(d,p) method for 1:1 adducts and scaled OVGF/6-31+G(d) method for 2:1 adducts.

Table S15. Relative energies of the studied amines and 2:1 complexes.[a]

No.	ΔE	No.	ΔE
1A	101.0	**6A**	3.5
1B	100.5	**6B**	5.3
1H	0.0	**6H**	0.0
2IAI	102.4	**7IAI**	4.4
2IBI	102.3	**7IBI**	7.1
2IHI	0.0	**7IHI**	0.0
3IAI	96.6	**8IAI**	23.9
3IBI	97.8	**8IBI**	23.6
3IHI	0.0	**8IHI**	3.1
3IAII	99.6	**8IAII**	17.0
3IBII	101.0	**8IBII**	16.4
3IHII	5.1	**8IHII**	7.6
3IIHI	2.1	**8IIHI**	0.0
3IIAII	102.1	**8IIAII**	8.6
3IIBII	102.1	**8IIBII**	12.6
3IIHII	0.4	**8IIHII**	1.3
4IAI	101.7	**9IAI**	5.9
4IBI	103.0	**9IBI**	9.9
4IHI	3.3	**9IHI**	4.1
4IAIV	100.0	**9IAIV**	3.3
4IBIV	100.2	**9IBIV**	7.7
4IHIV	1.0	**9IHIV**	2.1
4IVHI	3.3	**9IVHI**	1.2
4IVAIV	99.7	**9IVAIV**	3.6
4IVBIV	99.3	**9IVBIV**	6.5
4IVHIV	0.0	**9IVHIV**	0.0
5IAI	94.6	**10IAI**	0.5
5IBI	94.2	**10IBI**	2.9
5IHI	0.0	**10IHI**	0.0
5IAII	103.6	**10IAII**	15.7
5IBII	103.5	**10IBII**	15.3
5IHII	1.2	**10IHII**	1.7
5IIHI	11.7	**10IIHI**	10.9
5IIAII	111.6	**10IIAII**	30.2
5IIBII	112.2	**10IIBII**	29.9
5IIHII	15.6	**10IIHII**	12.6

[a] Energy values are in kJ/mol, calculations performed at B3LYP/6-311+G(2df,p) + ZPE level.

Table S16. Calculated complexation energies (in kJ/mol) of NH_3-TMA and methylamine-TMA systems.

		NH_3-TMA	**6**
method	basis set	$\Delta H_{complexation}$	
G3		102.5	115.2
B3LYP		75.7	80.0
B3PW88		80.0	83.7
PBE	6-31G*	81.6	86.8
BMK		85.0	93.5
TPSS		87.0	91.6
B3LYP		74.0	80.7
B3PW89		77.6	83.2
PBE	6-311+G(2df,p)/6-31G*	79.9	87.4
BMK		83.5	93.9
TPSS		84.5	91.1
B3LYP		73.6	79.9
B3PW90		77.3	82.9
PBE	(opt)[a] 6-311+G(2df,p)/6-31G*	79.4	87.0
BMK		83.3	93.7
TPSS		84.1	90.7
B3LYP		73.9	80.2
B3PW91		77.6	83.2
PBE	(opt)[a] 6-311+G(2df,p)/6-31+G**	71.7	79.3
BMK		83.5	93.6
TPSS		84.6	91.2
B3LYP		74.0	80.1
B3PW92		77.7	83.2
PBE	6-311+G(2df,p)	72.4	79.8
BMK		83.8	93.3
TPSS		84.6	91.2

[a] The geometry was optimized at 6-311+G(2df,p) level, only the (scaled) thermal correction was obtained at the calculation level employing the smaller basis set.

Table S17. Calculated OVGF Ionization Energies (in eV) for methylamine-TMA 1:1 adduct.

basis set	IE σ_{Al-C}	IE3
experimental	9.0	10.7
6-31G(d)	8.50	10.42
6-31G(d,p)	8.65	10.58
6-31G(2df,p)	8.77	10.66
6-31+G(d)	8.70	10.60
6-31+G(d,p)	8.84	10.75
6-31+G(2df,p)	8.96	10.82
6-31++G(d)	8.71	10.61
6-31++G(d,p)	8.85	10.76
6-31++G(2df,p)	8.97	10.83
6-311G(d)	8.73	10.60
6-311G(d,p)	8.90	10.78
6-311G(2df,p)	8.98	10.83
6-311+G(d)	8.78	10.65
6-311+G(d,p)	8.96	10.83
6-311+G(2df,p)	9.03	10.87
6-311++G(d)	8.78	10.65
6-311++G(d,p)	8.96	10.83
6-311++G(2df,p)	9.03	10.88

Cartesian coordinates of the optimized geometry of the calculated molecules

1

N	0.002105	0.000002	1.486587
C	0.010176	-0.000001	0.011762
B	1.473843	-0.000001	2.153360
H	-0.502084	0.814428	1.829787
H	-0.502090	-0.814419	1.829791
H	0.551260	0.884782	-0.323392
H	0.551254	-0.884789	-0.323388
H	-1.003418	0.000002	-0.396137
H	2.006909	-1.003783	1.756567
H	2.006914	1.003778	1.756565
H	1.293631	0.000000	3.343021

2I

N	1.450093	0.000007	3.590308
C	1.413514	0.000009	2.113234
C	-0.004431	-0.000002	1.540247
C	0.011716	-0.000001	0.006338
B	2.933621	0.000022	4.229377
H	0.950008	-0.814051	3.943039
H	0.949992	0.814055	3.943041
H	1.973582	0.879761	1.786310
H	1.973595	-0.879734	1.786308
H	-0.546648	0.881052	1.904258
H	-0.546634	-0.881064	1.904258
H	0.527457	0.884427	-0.378690
H	0.527471	-0.884421	-0.378691
H	-1.003758	-0.000008	-0.396064
H	3.461776	-1.003719	3.825759
H	3.461755	1.003776	3.825763
H	2.775709	0.000018	5.422500

2II

N	1.456425	0.008629	3.577870
C	1.426245	0.002206	2.094044
C	0.004623	0.073221	1.541046
C	0.010330	-0.006924	0.009205
B	0.949785	1.354237	4.323087
H	2.412715	-0.150401	3.886748
H	0.911538	-0.776764	3.930919
H	2.004309	0.870632	1.767721
H	1.925759	-0.903117	1.730031
H	-0.465131	1.000754	1.873036
H	-0.588993	-0.751602	1.954592
H	-1.006608	0.049812	-0.385347
H	0.583370	0.819740	-0.421401
H	0.455897	-0.943552	-0.340154
H	1.557612	2.255744	3.804082
H	1.245769	1.194291	5.479399
H	-0.237812	1.427295	4.162594

2III

N	2.182518	-1.213544	1.882514
C	1.397272	0.005284	2.172888
C	0.001519	0.001841	1.542856
C	0.015268	-0.020542	0.007750
B	3.640624	-1.261051	2.576260
H	2.308321	-1.310738	0.877253
H	1.659280	-2.033818	2.184712
H	1.991124	0.850548	1.815274
H	1.340075	0.082998	3.260514
H	-0.570209	-0.852402	1.926031
H	-0.519634	0.900050	1.889007
H	0.456392	-0.941339	-0.386742
H	0.585030	0.825017	-0.389813
H	-1.000141	0.042265	-0.390417
H	4.237535	-0.306976	2.148713
H	4.126273	-2.309553	2.237985
H	3.440063	-1.197766	3.761664

2IV

N	1.929156	1.352175	2.497348
C	1.396670	0.002464	2.174615
C	0.004630	0.047553	1.520595
C	0.035857	-0.020742	-0.012106
B	2.188940	2.386197	1.283112
H	2.818918	1.241441	2.979029
H	1.305430	1.805538	3.163289
H	1.365712	-0.579982	3.100702
H	2.122490	-0.462040	1.502291
H	-0.511253	0.959784	1.840941
H	-0.578614	-0.793159	1.908877
H	-0.978064	0.014578	-0.419316
H	0.606976	0.811109	-0.426568
H	0.497682	-0.956310	-0.342624
H	1.113723	2.693667	0.843760
H	2.756532	3.317710	1.793395
H	2.873158	1.795306	0.487200

2V

N	2.206236	-1.173356	1.716756
C	1.400790	-0.000420	2.143218
C	-0.001406	0.000835	1.533402
C	0.001470	-0.000988	-0.001112
B	1.641219	-2.634908	2.115317
H	3.135656	-1.094296	2.122696
H	2.338943	-1.144888	0.707305
H	1.340197	-0.049267	3.232437

H	1.934615	0.914674	1.861087
H	-0.554271	-0.864364	1.905680
H	-0.508488	0.898210	1.902609
H	0.619011	0.810625	-0.401691
H	0.369237	-0.952553	-0.397521
H	-1.011949	0.132200	-0.387097
H	0.672610	-2.841130	1.434471
H	2.541873	-3.394446	1.866836
H	1.387004	-2.576562	3.291270

3I

N	-0.005828	-0.000003	0.003105
C	1.239634	-0.000017	-0.775542
C	2.446347	-0.763479	-0.274071
C	2.446080	0.764131	-0.274456
B	0.012488	0.000004	1.627501
H	-0.555160	0.813683	-0.268404
H	-0.555160	-0.813704	-0.268361
H	1.059469	-0.000294	-1.846073
H	2.354245	-1.243121	0.691879
H	3.040827	-1.287864	-1.012516
H	2.353835	1.244215	0.691259
H	3.040384	1.288346	-1.013166
H	0.567619	1.004921	1.978505
H	-1.155598	0.000191	1.919776
H	0.567296	-1.005099	1.978484

3II

N	-0.004100	0.027887	-0.001934
C	1.315231	0.031178	-0.624865
C	1.473996	-0.369143	-2.080024
C	1.953380	-1.291110	-0.952787
B	0.010624	-0.030636	1.616717
H	-0.541961	-0.767166	-0.343214
H	-0.515379	0.861878	-0.286683
H	1.936213	0.820445	-0.218911
H	0.583411	-0.667559	-2.623419
H	2.212890	0.153626	-2.675325
H	1.373032	-2.185229	-0.751230
H	3.017167	-1.397500	-0.782055
H	0.632630	0.938189	1.967980
H	-1.147549	0.008923	1.943209
H	0.548396	-1.067257	1.902240

4I

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.483096
C	1.390423	0.000000	2.060137
C	1.876918	-0.978925	2.813306
B	-1.470323	-0.010907	-0.668225
H	0.500697	0.818185	-0.342416

H	0.520093	-0.810563	-0.331857
H	-0.565500	0.884353	1.789003
H	-0.562197	-0.880364	1.799979
H	2.010176	0.868059	1.836916
H	2.883228	-0.937958	3.216276
H	1.280481	-1.852866	3.060554
H	-2.015230	0.985205	-0.267874
H	-1.285566	-0.000939	-1.857239
H	-1.996360	-1.022727	-0.283182

4II

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.488836
C	1.400460	0.000000	2.037980
C	1.868735	-0.966100	2.819157
B	0.489431	1.364601	-0.721381
H	-0.946360	-0.179415	-0.328337
H	0.573417	-0.773685	-0.333285
H	-0.532097	0.907174	1.788894
H	-0.546326	-0.873884	1.856791
H	2.021966	0.847632	1.766671
H	2.878805	-0.931424	3.212992
H	1.258896	-1.821401	3.098434
H	1.646670	1.518088	-0.442131
H	-0.224556	2.228745	-0.280275
H	0.320426	1.173075	-1.897435

4III

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.487731
C	1.394571	0.000000	2.049250
C	1.833544	-0.882885	2.934495
B	0.441488	-1.382032	-0.715819
H	-0.937256	0.220263	-0.329449
H	0.602414	0.747967	-0.340395
H	-0.538943	0.888835	1.837891
H	-0.544238	-0.891381	1.804978
H	2.048997	0.804385	1.714797
H	2.837267	-0.823696	3.340517
H	1.208624	-1.703547	3.273541
H	1.586612	-1.578865	-0.417307
H	-0.312925	-2.215689	-0.282242
H	0.289078	-1.181509	-1.893701

4IV

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.470328
C	1.363923	0.000000	2.108192
C	2.533016	0.000000	1.478384
B	-1.474654	0.000000	-0.664066
H	0.505073	-0.815584	-0.341859

H	0.505073	0.815584	-0.341859
H	-0.573980	-0.875368	1.789918
H	-0.573980	0.875369	1.789918
H	1.347043	0.000000	3.196028
H	3.463736	0.000000	2.034108
H	2.619789	0.000000	0.395874
H	-1.290975	0.000000	-1.852758
H	-2.008728	-1.003441	-0.268305
H	-2.008728	1.003441	-0.268305

4V

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.480041
C	1.377300	0.000000	2.089945
C	2.535195	-0.124965	1.455188
B	0.040349	-1.455438	-0.714578
H	0.774633	0.571255	-0.334553
H	-0.846964	0.452408	-0.334140
H	-0.556175	-0.887343	1.798978
H	-0.539899	0.881017	1.845829
H	1.373117	0.125741	3.170428
H	3.468647	-0.090253	2.005540
H	2.606835	-0.301720	0.386926
H	1.013375	-2.022807	-0.302672
H	0.087473	-1.223354	-1.895239
H	-0.988091	-1.987478	-0.382956

5I

N	1.411530	-0.024430	3.215710
C	0.034969	-0.000080	2.672430
C	0.006454	-0.000057	1.207195
C	0.004846	-0.000120	0.011172
B	1.460285	-0.024676	4.830957
H	1.925618	0.781389	2.864013
H	1.896549	-0.848339	2.864640
H	-0.455203	0.889702	3.074404
H	-0.486598	-0.871541	3.075029
H	-0.008670	-0.000099	-1.054770
H	0.869469	-1.017664	5.167928
H	0.905274	0.989018	5.167147
H	2.626262	-0.045368	5.120798

5II

N	-0.299712	-1.336799	3.237078
C	0.053930	-0.006021	2.675136
C	-0.022503	-0.007576	1.215282
C	-0.048540	-0.012423	0.020662
B	-1.888156	-1.635870	3.342469
H	0.144205	-2.065040	2.680179
H	0.083396	-1.409467	4.177057
H	-0.655089	0.711886	3.095347
H	1.067109	0.273774	2.981163
H	-0.098780	-0.015029	-1.043950
H	-2.321577	-1.563200	2.226375
H	-1.967290	-2.739063	3.815982
H	-2.312671	-0.777329	4.073948

6

C	1.349969	1.905123	0.000000
Al	-0.131127	0.599235	0.000000
N	0.963874	-1.150139	0.000000
C	0.157404	-2.386690	0.000000
C	-1.140605	0.397828	-1.684783
C	-1.140605	0.397828	1.684783
H	-0.480617	-2.385442	-0.884454
H	1.575540	-1.129077	0.813094
H	1.575540	-1.129077	-0.813094
H	0.777258	-3.287007	0.000000
H	-0.480617	-2.385442	0.884454
H	-1.676070	1.323583	1.931770
H	-1.902278	-0.391258	1.648122
H	-0.496835	0.184781	2.549067
H	0.966847	2.933637	0.000000
H	1.998123	1.825582	0.882882
H	1.998123	1.825582	-0.882882
H	-1.676070	1.323583	-1.931770
H	-0.496835	0.184781	-2.549067
H	-1.902278	-0.391258	-1.648122

7I

C	-0.019381	-0.077479	0.039434
Al	0.055470	0.021165	2.011100
N	2.104708	0.078502	2.266033
C	2.577720	0.015015	3.664499
C	4.094865	0.154104	3.811631
C	4.533959	0.044041	5.277052
C	-0.407493	-1.624277	2.999147
C	-0.458392	1.743723	2.832649
H	2.235251	-0.938395	4.076438
H	2.434674	0.937059	1.827369
H	2.511962	-0.684121	1.727219
H	2.064238	0.807365	4.217234
H	-1.513674	1.968571	2.630498
H	-0.348657	1.761680	3.924330
H	0.109752	2.596067	2.435799
H	-1.058363	-0.110829	-0.312619
H	0.442249	0.785007	-0.458942
H	0.463723	-0.978209	-0.362241
H	-1.454569	-1.902914	2.822823
H	0.189565	-2.493979	2.692972
H	-0.299281	-1.524621	4.086588
H	4.590316	-0.621794	3.215644
H	5.615900	0.161351	5.372013

H	4.056073	0.815425	5.888023
H	4.410431	1.120698	3.400807
H	4.262791	-0.930646	5.693067

7II

C	0.061457	-0.273206	0.060123
Al	-0.006419	0.126093	1.995876
N	2.026374	0.421437	2.286999
C	2.624556	0.106890	3.605233
C	2.115979	1.056341	4.688857
C	2.760296	0.749850	6.045944
C	-0.365998	-1.397108	3.199292
C	-0.785697	1.874570	2.479703
H	2.345945	-0.921449	3.850557
H	2.230769	1.389377	2.041703
H	2.462628	-0.147148	1.563454
H	3.718384	0.158096	3.548093
H	-1.843025	1.914969	2.186610
H	-0.756756	2.095109	3.553639
H	-0.301496	2.716292	1.966345
H	-0.945072	-0.425953	-0.349644
H	0.504482	0.541303	-0.528989
H	0.625576	-1.185527	-0.175949
H	-1.414510	-1.710821	3.113067
H	0.234253	-2.284793	2.959671
H	-0.203394	-1.175197	4.261891
H	1.028170	0.970195	4.760038
H	2.394347	1.434370	6.814467
H	2.526486	-0.269588	6.366520
H	2.334761	2.090873	4.396647
H	3.849282	0.847208	5.998811

7III

C	0.156488	0.271986	0.071977
Al	-0.002016	0.096727	2.033667
C	1.686226	-0.033744	3.049626
C	-1.542824	-0.945559	2.697160
N	-0.601999	2.016255	2.492072
C	-0.832883	2.290215	3.926652
H	0.116627	2.112311	4.440009
H	-1.452711	2.200587	1.961842
H	0.102080	2.652560	2.123129
C	-1.348283	3.703044	4.222508
H	-1.543064	1.540858	4.284675
H	-1.481740	-1.987943	2.358534
H	-1.609321	-0.985476	3.791645
H	-2.506663	-0.567936	2.329284
H	0.490136	-0.672099	-0.377825
H	-0.795198	0.518212	-0.417451
H	0.886577	1.029874	-0.241471
H	2.197401	-0.978711	2.824059
H	2.402131	0.762035	2.804104
H	1.546056	-0.018924	4.137922
C	-0.366907	4.813207	3.823204
H	-1.552523	3.764288	5.296485
H	-0.753552	5.794205	4.108969
H	0.600838	4.677026	4.315810
H	-2.309909	3.850865	3.716022
H	-0.196787	4.839143	2.742415

7IV

C	0.150909	-0.298185	-0.031790
Al	-0.146966	0.080931	1.888045
N	1.844976	0.513328	2.348466
C	2.535145	-0.027886	3.550560
C	2.477663	0.935516	4.738108
C	1.061902	1.224918	5.250874
C	-0.544528	-1.484185	3.020780
C	-1.105329	1.772284	2.242627
H	2.055249	-0.976179	3.806044
H	1.972963	1.523560	2.307138
H	2.291511	0.147290	1.509809
H	3.582533	-0.232160	3.307411
H	-1.958495	1.859521	1.556902
H	-1.514716	1.856432	3.255796
H	-0.493992	2.668673	2.068194
H	-0.792901	-0.532509	-0.540367
H	0.580118	0.554446	-0.576294
H	0.809947	-1.159053	-0.210669
H	-1.540254	-1.877034	2.775580
H	0.153898	-2.316776	2.864431
H	-0.559238	-1.268609	4.095832
H	3.076890	0.494836	5.541486
H	1.098262	1.879403	6.125340
H	0.447691	1.714597	4.491418
H	2.977855	1.872923	4.462151
H	0.558049	0.298908	5.540343

7V

C	-0.027816	-0.238402	0.030154
Al	0.014057	0.117637	1.973294
N	2.065974	0.305591	2.188272
C	2.691007	-0.032196	3.489972
C	2.235401	0.911914	4.605073
C	2.585855	2.383464	4.344791
C	-0.376353	-1.420418	3.146970
C	-0.657291	1.889354	2.533778
H	2.395612	-1.056404	3.727993
H	2.316619	1.256787	1.923605
H	2.450015	-0.293141	1.459531
H	3.783387	-0.000485	3.398884
H	-1.735962	1.963338	2.342217
H	-0.521443	2.105571	3.600611
H	-0.198896	2.717369	1.975810

H	-1.059628	-0.347302	-0.327813
H	0.414940	0.567710	-0.570107
H	0.486183	-1.168178	-0.249007
H	-1.428198	-1.718039	3.045728
H	0.212887	-2.312558	2.895565
H	-0.218066	-1.221290	4.214393
H	2.716623	0.576402	5.529180
H	2.347999	2.994010	5.219035
H	3.653628	2.506180	4.133117
H	1.156302	0.804789	4.750102
H	2.012556	2.793907	3.508076

8I

C	-1.217219	2.544577	0.000000
Al	0.177752	1.142290	0.000000
C	1.175642	0.947482	1.691874
C	1.175642	0.947482	-1.691874
N	-1.190825	-0.442884	0.000000
C	-0.902751	-1.873988	0.000000
C	0.303559	-2.383594	0.763038
H	-1.766006	-0.216330	-0.811225
H	-1.766006	-0.216330	0.811225
H	-1.786522	-2.505475	0.000000
C	0.303559	-2.383594	-0.763038
H	1.533409	1.931208	-2.023412
H	2.064300	0.309432	-1.615217
H	0.566521	0.555417	-2.517131
H	-0.751193	3.538588	0.000000
H	-1.869944	2.521498	-0.883060
H	-1.869944	2.521498	0.883060
H	1.533409	1.931208	2.023412
H	0.566521	0.555417	2.517131
H	2.064300	0.309432	1.615217
H	0.200576	-3.328598	1.282788
H	0.923008	-1.646215	1.258704
H	0.200576	-3.328598	-1.282788
H	0.923008	-1.646215	-1.258704

8II

C	-0.034791	-0.111746	0.039186
Al	-0.018289	-0.050618	2.011036
C	1.741706	-0.053238	2.905607
N	-0.695567	-1.953952	2.470171
C	0.225005	-3.041088	2.162857
C	0.173441	-3.657267	0.787692
C	-0.276248	-4.466588	2.008978
C	-1.453377	0.992985	2.880092
H	1.197902	-2.880574	2.612724
H	-1.341007	-4.638855	2.128072
H	0.356939	-5.273113	2.359001
H	-0.594210	-3.296352	0.111003
H	1.110087	-3.913521	0.308359
H	-1.571457	-2.084611	1.966258
H	-0.934932	-1.966531	3.460951
H	0.238086	0.861396	-0.388997
H	-1.021483	-0.357419	-0.376412
H	0.678353	-0.838419	-0.369802
H	-1.304564	2.068928	2.722337
H	-1.498225	0.849836	3.967777
H	-2.452019	0.766498	2.483285
H	2.145350	0.965030	2.975303
H	2.498035	-0.646314	2.376381
H	1.698870	-0.429390	3.937005

9I

C	-0.019096	0.005457	0.027345
Al	0.039096	-0.012640	2.000336
N	2.089286	-0.026362	2.268483
C	2.545310	-0.066833	3.678428
C	4.045196	-0.057732	3.813779
C	4.744914	-1.034846	4.377506
C	-0.470556	-1.693228	2.901831
C	-0.424261	1.678951	2.909134
H	2.120876	-0.963569	4.135145
H	2.453797	0.806711	1.808657
H	2.481318	-0.818733	1.761867
H	2.103840	0.801058	4.177659
H	-1.475191	1.939591	2.728897
H	-0.304727	1.641645	3.999291
H	0.162315	2.535350	2.549456
H	-1.052661	0.065368	-0.337026
H	0.502723	0.868755	-0.406848
H	0.411932	-0.895030	-0.429312
H	-1.531140	-1.919709	2.732908
H	0.086661	-2.564499	2.532122
H	-0.337881	-1.662342	3.990680
H	4.560055	0.818518	3.420485
H	5.825111	-0.983714	4.461316
H	4.258520	-1.917268	4.784470

9II

C	-0.045879	0.057968	0.038368
Al	0.015784	-0.064802	2.008926
C	1.817568	-0.099393	2.818074
N	-0.676504	-2.016376	2.167616
C	-1.191479	-2.504571	3.472223
C	-0.067395	-2.680644	4.456497
C	0.199954	-3.831266	5.061631
C	-1.400057	0.883448	3.006001
H	-1.895165	-1.748609	3.834006
H	0.043434	-2.652846	1.828007
H	-1.424363	-2.042289	1.476042
H	-1.730820	-3.449279	3.348297
H	2.413464	0.744248	2.445587

H	1.814389	-0.009217	3.911112
H	2.389523	-1.003982	2.571755
H	0.298739	1.041148	-0.306646
H	0.599141	-0.678514	-0.459395
H	-1.056253	-0.067629	-0.373814
H	-1.294222	1.969866	2.889682
H	-2.414119	0.641841	2.659305
H	-1.375940	0.692711	4.086921
H	0.533306	-1.797414	4.660486
H	1.008063	-3.917817	5.779946
H	-0.385994	-4.726118	4.868535

9III

C	-0.003908	-0.009045	0.043085
Al	-0.012143	0.054649	2.019295
C	1.755853	0.073978	2.891783
N	-0.638667	2.026720	2.212038
C	-1.320738	2.450329	3.461665
C	-0.373910	2.429396	4.630901
C	-0.607184	1.774105	5.759427
C	-1.475179	-0.909396	2.928811
H	-1.254971	2.181660	1.415962
H	0.177005	2.616011	2.049356
H	-1.728441	3.461134	3.335234
H	-2.151383	1.763800	3.636330
H	0.540900	3.010702	4.520109
H	-1.503929	1.176097	5.893345
H	0.093589	1.807728	6.586374
H	0.642700	0.755747	-0.408439
H	-1.001338	0.109243	-0.401362
H	0.375478	-0.972862	-0.319690
H	-2.470324	-0.668852	2.531117
H	-1.356692	-1.993941	2.807768
H	2.270011	-0.886459	2.756669
H	2.430838	0.837235	2.481357
H	1.691541	0.244741	3.972888
H	-1.502011	-0.724041	4.010134

9IV

C	-2.646483	1.503092	0.000000
Al	-1.505059	-0.108758	0.000000
N	0.346966	0.809709	0.000000
C	1.502262	-0.099455	0.000000
C	2.854712	0.567312	0.000000
C	3.087964	1.873943	0.000000
C	-1.412456	-1.130442	-1.687234
C	-1.412456	-1.130442	1.687234
H	1.408267	-0.750070	-0.875869
H	0.385719	1.420865	0.814342
H	0.385719	1.420865	-0.814342
H	1.408267	-0.750070	0.875869
H	-2.394344	-1.551032	1.940244
H	-0.720983	-1.981789	1.649709
H	-1.119898	-0.514701	2.548533
H	-3.709750	1.230853	0.000000
H	-2.498224	2.138794	0.882927
H	-2.498224	2.138794	-0.882927
H	-2.394344	-1.551032	-1.940244
H	-1.119898	-0.514701	-2.548533
H	-0.720983	-1.981789	-1.649709
H	3.694293	-0.124876	0.000000
H	4.101079	2.259721	0.000000
H	2.291673	2.612045	0.000000

9V

C	0.075326	0.143740	0.053002
Al	-0.001889	0.061500	2.021502
C	1.709601	0.026609	3.008482
N	-0.817966	1.922263	2.518982
C	-0.918704	2.988076	1.502678
C	0.372628	3.726546	1.280075
C	1.533487	3.488272	1.877100
C	-1.447240	-1.033326	2.814316
H	-0.355468	2.286613	3.350879
H	-1.753599	1.650959	2.814314
H	-1.236201	2.522432	0.564045
H	-1.692303	3.713900	1.783912
H	0.298123	4.532721	0.553572
H	2.404324	4.091994	1.647292
H	1.675932	2.680947	2.588206
H	1.653429	0.493504	4.001941
H	2.020077	-1.011149	3.186914
H	2.535915	0.507620	2.471891
H	-1.581449	-0.851506	3.889715
H	-1.234827	-2.105526	2.717119
H	-2.424003	-0.876375	2.336184
H	0.528300	-0.773197	-0.346069
H	0.691346	0.973784	-0.315550
H	-0.909538	0.227605	-0.424279

10I

C	-2.274358	1.727248	0.000000
Al	-1.388427	-0.035608	0.000000
N	0.587782	0.589552	0.000000
C	1.580135	-0.507084	0.000000
C	2.966240	-0.027097	0.000000
C	4.084513	0.397561	0.000000
C	-1.434447	-1.061951	-1.686058
C	-1.434447	-1.061951	1.686058
H	1.391077	-1.126249	-0.880830
H	0.738976	1.184470	0.813071
H	0.738976	1.184470	-0.813071
H	1.391077	-1.126249	0.880830
H	-2.465519	-1.341117	1.938983

H	-0.870711	-2.002883	1.648992
H	-1.059028	-0.493918	2.547942
H	-3.366241	1.615900	0.000000
H	-2.032670	2.333197	0.882955
H	-2.032670	2.333197	-0.882955
H	-2.465519	-1.341117	-1.938983
H	-1.059028	-0.493918	-2.547942
H	-0.870711	-2.002883	-1.648992
H	5.085037	0.765325	0.000000

10II

C	0.185348	0.021035	0.046083
Al	-0.068772	-0.045381	2.004988
C	1.566330	-0.090137	3.109231
N	-0.669393	-2.049764	2.116643
C	-0.266092	-2.843502	3.302448
C	-0.982492	-2.398995	4.498470
C	-1.586385	-2.045410	5.467124
C	-1.639541	0.900492	2.722426
H	-0.457489	-3.910575	3.144890
H	-0.280784	-2.477179	1.277736
H	-1.682785	-2.078428	2.016103
H	0.808347	-2.701882	3.445163
H	2.059293	0.890658	3.100629
H	1.364606	-0.319754	4.163484
H	2.319707	-0.806321	2.754658
H	0.446438	1.034350	-0.284643
H	0.996691	-0.629835	-0.307150
H	-0.717881	-0.253717	-0.515513
H	-1.524958	1.987591	2.622637
H	-2.570290	0.645308	2.198499
H	-1.801283	0.698338	3.787733
H	-2.114066	-1.715332	6.332400

1A

B	2.019749	0.017869	2.225614
H	1.617110	0.039207	3.350489
H	2.205623	-1.026416	1.672757
H	2.239311	1.040811	1.645741
N	4.070779	-0.006605	2.923001
C	4.998726	-0.030285	1.799099
H	4.196308	0.816907	3.500634
H	4.173176	-0.822516	3.515791
H	4.814890	0.847804	1.175686
H	4.788982	-0.913606	1.191427
H	6.056659	-0.043253	2.089552
N	-0.007080	0.040656	1.461215
C	-0.008242	0.022313	0.003610
H	-0.453648	0.872808	1.829603
H	-0.481225	-0.766437	1.850341
H	0.522790	-0.870367	-0.334966
H	0.547395	0.890983	-0.357136
H	-1.009262	0.030707	-0.445424

1B

B	2.010007	-0.008126	2.219816
H	1.607176	0.049635	3.344170
H	2.229649	0.994995	1.607176
H	2.193890	-1.072933	1.706344
N	-0.014033	-0.009818	1.452816
C	-0.007948	0.015487	-0.004906
H	-0.485419	0.798294	1.843150
H	-0.466361	-0.841336	1.815663
H	0.559770	-0.844720	-0.367328
H	0.514166	0.916527	-0.334402
H	-1.006483	-0.001805	-0.459049
N	4.041015	-0.040715	2.967731
C	4.221807	-1.138643	3.909780
H	4.219593	0.859828	3.397538
H	4.649243	-0.128692	2.161505
H	3.522282	-1.004447	4.737859
H	5.238301	-1.221391	4.314151
H	3.963543	-2.074907	3.409466

1H

B	-0.452529	0.014839	-0.830149
H	-0.258173	-0.592265	0.195054
H	0.548272	0.139998	-1.489803
H	-1.373456	-0.438835	-1.465717
N	-0.912880	1.486282	-0.381731
C	0.076980	2.215100	0.426573
H	-1.787039	1.379163	0.154089
H	-1.141308	2.025867	-1.212898
H	-0.287123	3.206825	0.707190
H	0.281973	1.629139	1.322982
H	1.001342	2.303797	-0.145609
N	-3.473416	1.172528	1.187458
C	-3.423747	-0.287140	1.366943
H	-4.270309	1.429910	0.613747
H	-3.598121	1.638511	2.080136
H	-4.343945	-0.712175	1.785107
H	-2.591903	-0.536552	2.028544
H	-3.216565	-0.757591	0.403134

2IAI

B	3.565444	0.001531	4.272034
H	3.184642	0.005457	5.404477
H	3.758632	1.033377	3.700241
H	3.754726	-1.034211	3.706038
N	5.632772	0.000158	4.953723
C	6.579980	-0.003985	3.846604
C	8.061856	-0.005917	4.247640
C	8.991452	-0.010814	3.027468

H	5.741131	-0.818135	5.543902
H	5.742704	0.821680	5.539093
H	6.362547	0.872004	3.225567
H	6.359254	-0.881755	3.229236
H	8.266516	0.874718	4.868486
H	8.263016	-0.884272	4.872848
H	10.042442	-0.011758	3.327667
H	8.820978	0.871521	2.402790
H	8.818004	-0.895971	2.407621
N	1.505972	0.003566	3.566180
C	1.420088	-0.001095	2.111690
C	-0.003028	0.001446	1.535914
C	-0.006570	-0.003917	0.001979
H	1.061984	-0.813990	3.971305
H	1.065746	0.825820	3.965876
H	1.965976	-0.880943	1.753640
H	1.971559	0.872802	1.747650
H	-0.543960	-0.874998	1.912865
H	-0.538307	0.883981	1.906681
H	-1.025418	-0.002186	-0.393806
H	0.509132	0.876868	-0.393074
H	0.503698	-0.890614	-0.386860

2IBI

B	3.584406	0.021244	4.226733
H	3.780643	-0.990207	3.621256
H	3.741224	1.078234	3.690383
H	3.234409	-0.021703	5.368637
N	1.515196	0.006134	3.563356
C	1.422667	-0.000803	2.109374
C	-0.000799	-0.001379	1.534245
C	0.000797	0.000836	0.000253
H	1.074827	-0.811344	3.972530
H	1.077972	0.829157	3.964797
H	1.972385	0.872867	1.742205
H	1.968859	-0.880944	1.752822
H	-0.540381	0.877622	1.907091
H	-0.538725	-0.882052	1.905490
H	0.505007	0.890992	-0.388374
H	0.526027	-0.876520	-0.389719
H	-1.016106	-0.011741	-0.400298
N	5.662685	0.059553	4.880929
C	5.938339	1.217442	5.721238
C	7.380655	1.335768	6.233957
C	7.577843	2.576589	7.114190
H	6.236518	0.057279	4.043968
H	5.828469	-0.811714	5.374059
H	5.673799	2.110506	5.144358
H	5.244362	1.180847	6.568178
H	7.634620	0.432494	6.801712
H	8.065363	1.372467	5.377997
H	7.343638	3.489790	6.558328
H	8.608592	2.655000	7.469255
H	6.922394	2.542725	7.989978

2IHI

B	2.931345	0.034753	4.222623
H	2.766099	0.091671	5.418026
H	3.477704	1.023074	3.793463
H	3.482416	-0.980502	3.883341
N	1.463384	0.022588	3.576192
C	1.426386	0.001317	2.102096
C	0.003299	-0.005061	1.541488
C	0.000204	-0.011068	0.007621
H	0.986385	0.869072	3.924963
H	0.953106	-0.780809	3.937345
H	1.976143	0.882251	1.759911
H	1.987137	-0.877594	1.771490
H	-0.533330	-0.885364	1.915683
H	-0.534334	0.875440	1.912033
H	0.518445	0.868196	-0.386413
H	0.506038	-0.899718	-0.381512
H	-1.019454	-0.004148	-0.384713
N	0.903123	2.552211	4.988398
C	0.417469	2.237709	6.333667
C	0.777904	3.260327	7.420253
C	0.239196	2.848580	8.796137
H	1.921228	2.563942	4.979383
H	0.586360	3.471888	4.697286
H	0.826625	1.258892	6.607381
H	-0.672290	2.128019	6.286203
H	1.867928	3.367092	7.461485
H	0.372739	4.240169	7.139014
H	0.662380	1.888975	9.108187
H	-0.850133	2.742628	8.774306
H	0.487777	3.589027	9.560579

3IAI

B	-0.006394	0.009725	1.051774
H	0.070837	-0.023691	-0.138183
H	0.984214	0.061915	1.706038
H	-1.075546	-0.012273	1.570954
N	0.113033	-2.251834	0.974677
C	-0.009462	-3.120085	2.120005
C	-1.048523	-2.757530	3.164990
C	0.437752	-2.574557	3.464240
H	-0.583070	-2.468850	0.268745
H	1.028537	-2.332786	0.544496
H	0.154295	-4.183724	1.952134
H	0.912283	-3.258079	4.158423
H	0.813169	-1.558655	3.468760
H	-1.578418	-3.566046	3.654724
H	-1.625228	-1.859084	2.982398
N	-0.122288	2.260226	0.855487
C	0.007852	3.169380	1.968021

C	1.081373	2.865689	2.996360
C	-0.392150	2.660040	3.341210
H	0.565330	2.455364	0.135066
H	-1.042840	2.320198	0.432870
H	-0.184888	4.222711	1.769138
H	-0.863826	3.355994	4.024928
H	-0.743506	1.636702	3.390056
H	1.605418	3.701664	3.444439
H	1.671614	1.973022	2.828763

3IBI

B	0.006456	-0.042369	1.168744
H	-0.289282	-0.119355	0.018635
H	1.148984	0.018639	1.490313
H	-0.850227	-0.027463	1.994581
N	-0.083269	2.212401	0.904780
C	0.069935	3.164928	1.976845
C	0.955699	2.769634	3.144727
C	-0.560827	2.821290	3.314121
H	-0.975588	2.323327	0.434429
H	0.649763	2.313542	0.210544
H	0.073342	4.219281	1.703861
H	1.405792	1.785633	3.093342
H	1.554413	3.542043	3.613050
H	-1.076276	1.870580	3.374708
H	-0.989508	3.628695	3.895935
N	0.015165	-2.302356	1.408470
C	0.797587	-3.204765	0.600091
C	2.118207	-2.691640	0.054634
C	0.925819	-2.887265	-0.878741
H	-0.975711	-2.512113	1.345778
H	0.283085	-2.351901	2.385860
H	0.762075	-4.260931	0.863614
H	2.376070	-1.670026	0.306227
H	2.945902	-3.388004	-0.011723
H	0.945004	-3.716176	-1.576391
H	0.426633	-1.990510	-1.224964

3IHI

B	1.777719	-2.633523	0.285518
H	1.609179	-2.610060	-0.907792
H	2.656652	-3.399846	0.597160
H	0.762493	-2.842450	0.893473
N	2.351405	-1.184930	0.704112
C	1.502323	0.007537	0.626498
C	0.273256	0.023768	-0.257653
C	0.127057	-0.003394	1.262189
H	2.702736	-1.261753	1.656637
H	3.175203	-1.056525	0.094866
H	2.069587	0.930104	0.701444
H	0.034887	-0.892838	-0.781628
H	0.053621	0.943862	-0.786087
H	-0.205833	-0.939221	1.694044
H	-0.191630	0.897107	1.773504
N	4.464485	-1.570353	-1.358853
C	4.396517	-0.919100	-2.643387
C	3.161733	-0.084239	-2.925403
C	4.503828	0.596042	-2.664052
H	3.947022	-2.447762	-1.367845
H	5.425124	-1.778773	-1.104989
H	4.826678	-1.445066	-3.494001
H	2.412042	-0.043114	-2.142798
H	2.770248	-0.077000	-3.935617
H	4.636669	1.086406	-1.706543
H	5.014358	1.063554	-3.497740

3IAII

B	0.069297	-0.066593	0.990294
H	0.072880	-0.327691	-0.174110
H	-0.032985	1.067649	1.342553
H	0.117903	-0.939270	1.797407
N	2.270292	0.123982	0.856285
C	3.138289	0.241668	2.003136
C	2.855422	-0.654545	3.194477
C	2.557162	0.840451	3.272280
H	2.525382	-0.670341	0.278537
H	2.308071	0.956245	0.277090
H	4.186919	0.457356	1.803277
H	1.513901	1.128938	3.232191
H	3.201132	1.466419	3.878747
H	2.001454	-1.315528	3.110330
H	3.702653	-1.043983	3.746629
N	-2.180661	-0.210053	1.003479
C	-2.703037	0.080502	2.310453
C	-3.032550	-1.060463	3.241487
C	-4.158588	-0.176789	2.694755
H	-2.424896	-1.143363	0.691493
H	-2.502561	0.454976	0.307924
H	-2.223592	0.946852	2.755351
H	-4.802879	-0.608879	1.936536
H	-4.647665	0.513060	3.373226
H	-2.949221	-2.065723	2.841547
H	-2.759305	-0.970273	4.285761

3IBII

B	1.241533	-3.244374	0.577552
H	2.351024	-3.664451	0.711935
H	0.545357	-3.098895	1.532425
H	0.824126	-3.030316	-0.516058
N	2.100565	-1.212480	0.730433
C	1.322004	0.002322	0.759548
C	0.034771	-0.004023	1.564508
C	-0.014099	0.003393	0.038845
H	2.705125	-1.244244	-0.083895

H	2.684998	-1.296575	1.555805
H	1.876761	0.939344	0.747649
H	-0.300409	-0.923049	-0.443550
H	-0.318578	0.913409	-0.464601
H	-0.232395	0.902006	2.095515
H	-0.224522	-0.934190	2.055393
N	0.538712	-5.387666	0.404769
C	1.096547	-6.016109	-0.760918
C	0.253022	-6.132527	-2.006433
C	0.659423	-7.397615	-1.241657
H	0.851913	-5.827789	1.263622
H	-0.475041	-5.389029	0.394576
H	2.140609	-5.755107	-0.904742
H	-0.783383	-5.818767	-1.935364
H	0.715173	-5.932806	-2.965484
H	1.400592	-8.052756	-1.685401
H	-0.112759	-7.900887	-0.669638

3IHII

B	1.944222	-2.583251	0.166582
H	0.905699	-2.901777	0.679172
H	2.848039	-3.318303	0.480906
H	1.855174	-2.476839	-1.031930
N	2.383812	-1.140578	0.733353
C	1.459393	-0.004637	0.660877
C	0.048775	-0.150222	1.195814
C	0.296613	-0.027925	-0.306257
H	2.656186	-1.267207	1.706202
H	3.247759	-0.912885	0.215652
H	1.952626	0.948034	0.824691
H	-0.240754	-1.129918	1.556357
H	-0.371083	0.694561	1.728735
H	0.171212	-0.931182	-0.889518
H	0.042121	0.900697	-0.802683
N	4.687186	-1.234538	-1.136067
C	4.700490	-0.399220	-2.313386
C	3.521797	-0.459236	-3.257435
C	4.893819	-0.969045	-3.714372
H	5.631185	-1.500064	-0.870824
H	4.171473	-2.096015	-1.307983
H	5.127171	0.580876	-2.125084
H	2.759809	-1.201748	-3.042042
H	3.149639	0.465962	-3.680714
H	5.018405	-2.043355	-3.799456
H	5.441952	-0.383887	-4.444271

3IIHI

B	3.161916	-1.470794	-0.106178
H	3.944414	-0.561509	0.026331
H	3.643269	-2.537472	0.186641
H	2.643128	-1.479940	-1.191969
N	1.995913	-1.213213	0.970786
C	1.290687	0.051050	0.813374
C	0.090483	0.104594	-0.094537
C	-0.089603	0.233401	1.421521
H	1.329531	-1.980669	0.908312
H	2.407250	-1.249633	1.918533
H	1.979082	0.887701	0.806531
H	-0.215583	-0.824379	-0.563949
H	-0.044681	0.984550	-0.710923
H	-0.523687	-0.611838	1.945559
H	-0.347088	1.201683	1.834092
N	3.211364	-1.101979	3.759972
C	4.435748	-1.836938	3.997532
C	4.628633	-3.159236	3.275623
C	5.436878	-1.934574	2.861290
H	2.499439	-1.373760	4.432574
H	3.370217	-0.105818	3.885274
H	4.853389	-1.775358	5.000959
H	5.125448	-3.961903	3.807882
H	3.848153	-3.467372	2.588553
H	5.161531	-1.478905	1.915700
H	6.490105	-1.898271	3.113422

3IIAII

B	3.743259	0.852042	-0.834346
H	4.172069	1.947805	-0.631273
H	4.148282	-0.073161	-0.195720
H	2.913240	0.675102	-1.671008
N	5.328534	0.471533	-2.316219
C	5.171434	-0.833594	-2.897397
C	4.481711	-0.962710	-4.232785
C	5.972207	-1.297698	-4.112263
H	5.278759	1.209904	-3.009289
H	6.203903	0.562692	-1.811433
H	4.930048	-1.583425	-2.150524
H	6.675886	-0.593809	-4.543625
H	6.271059	-2.338265	-4.170255
H	4.215627	-0.043569	-4.744505
H	3.776843	-1.773197	-4.371941
N	2.168461	1.153357	0.676662
C	1.314555	-0.000331	0.751978
C	0.006722	0.006055	0.000310
C	0.001998	-0.005940	1.532764
H	1.659582	1.992584	0.422051
H	2.656064	1.325565	1.549606
H	1.881539	-0.925820	0.734481
H	-0.276894	0.929679	-0.493605
H	-0.288176	-0.892869	-0.527014
H	-0.282183	0.912078	2.035944
H	-0.297142	-0.917155	2.038395

3IIBII

B	3.809625	-0.800271	2.294592

H	4.154470	0.132479	1.635373
H	4.251936	-1.885966	2.066457
H	3.025180	-0.645738	3.179725
N	5.484017	-0.453629	3.687849
C	6.756566	-0.591962	3.033536
C	7.490921	0.648471	2.586659
C	8.072749	-0.214813	3.710078
H	5.355169	-1.142593	4.421453
H	5.355680	0.468926	4.088543
H	6.774668	-1.439801	2.355882
H	8.016989	0.179670	4.719047
H	8.954398	-0.809382	3.498600
H	7.977531	0.640558	1.618922
H	7.060928	1.605649	2.862866
N	2.158766	-1.148747	0.868645
C	1.300302	0.001342	0.785594
C	-0.008584	-0.001019	1.537614
C	-0.010663	-0.005743	0.005061
H	1.660582	-1.981027	1.163704
H	2.621594	-1.345262	-0.012640
H	1.864444	0.928802	0.792048
H	-0.292051	-0.920096	2.039878
H	-0.306830	0.902263	2.055847
H	-0.290496	-0.931123	-0.487081
H	-0.313050	0.897581	-0.512505

3IIHII

B	3.504597	-0.387858	0.456013
H	3.303118	-0.482898	-0.724858
H	4.386457	-1.120746	0.835968
H	3.682308	0.753913	0.808028
N	2.176051	-0.881187	1.215697
C	0.975093	-0.118888	0.903937
C	0.133261	-0.540635	-0.271820
C	-0.395877	-0.720152	1.155131
H	2.021078	-1.863695	0.998220
H	2.378506	-0.818237	2.226760
H	1.124231	0.940264	1.075923
H	0.445174	-1.429330	-0.810150
H	-0.299100	0.233091	-0.893874
H	-0.437822	-1.730838	1.547531
H	-1.186785	-0.066635	1.503257
N	3.565635	-0.283134	3.755111
C	4.147867	-1.314206	4.580604
C	5.137674	-2.272812	3.957783
C	5.607052	-1.277149	5.023377
H	4.200457	-0.011078	3.005750
H	3.372459	0.550400	4.302595
H	3.438603	-1.733609	5.287272
H	5.080727	-3.321473	4.224698
H	5.425725	-2.079035	2.929337
H	6.205505	-0.436852	4.687834
H	5.861905	-1.658339	6.005910

4IAI

B	3.280776	-1.105202	4.108357
H	2.957652	-2.038335	4.779118
H	3.839073	-1.278053	3.065480
H	3.048262	0.008740	4.474706
N	5.215490	-1.019292	5.103945
C	6.083828	-0.032286	4.464337
C	7.401740	0.184184	5.167249
C	7.802135	1.347718	5.667671
H	5.051605	-0.789399	6.078821
H	5.610356	-1.953092	5.064950
H	6.250664	-0.371773	3.436392
H	5.530226	0.909537	4.403327
H	8.039782	-0.693627	5.270400
H	8.755086	1.452933	6.175548
H	7.187095	2.239613	5.581145
N	1.363500	-1.143084	3.076557
C	1.234275	0.005264	2.181024
C	-0.011984	-0.007655	1.329844
C	-0.012435	-0.020205	0.001540
H	1.305646	-2.017728	2.564928
H	0.642095	-1.150011	3.789991
H	2.124422	0.034582	1.545410
H	1.259419	0.903476	2.807391
H	-0.959824	-0.023257	1.868037
H	-0.935234	-0.040422	-0.568687
H	0.916679	-0.006125	-0.562187

4IBI

B	3.295081	-1.130277	4.083507
H	2.990192	-2.101306	4.709163
H	3.839791	-1.243042	3.026183
H	3.054532	-0.042267	4.516881
N	1.370479	-1.145859	3.071387
C	1.240682	0.005349	2.179570
C	-0.003677	-0.006871	1.325761
C	-0.001781	-0.016619	-0.002599
H	0.648942	-1.155349	3.784785
H	1.311894	-2.018442	2.556182
H	2.131958	0.039399	1.545645
H	1.263332	0.901815	2.808563
H	-0.953093	-0.024357	1.861190
H	-0.923345	-0.033683	-0.574764
H	0.929093	-0.000598	-0.563542
N	5.217546	-1.102794	5.100037
C	5.045699	-0.887948	6.535910
C	6.318684	-1.002382	7.338395
C	6.515137	-1.885287	8.311289
H	5.667087	-1.993375	4.912804
H	5.779009	-0.373603	4.672625
H	4.604098	0.106697	6.660274

H	4.307302	-1.610712	6.896164
H	7.118891	-0.312337	7.070270
H	5.736045	-2.585957	8.600281
H	7.451850	-1.935412	8.856269

4IHI

B	2.628333	-1.247681	3.991454
H	3.578300	-1.293748	3.253943
H	2.511790	-2.246259	4.659172
H	2.618047	-0.244621	4.665132
N	1.313976	-1.174888	3.074350
C	1.251387	0.002360	2.180076
C	0.010965	0.002891	1.327013
C	0.023704	-0.001489	-0.000484
H	0.509205	-1.156161	3.720207
H	1.241969	-2.021835	2.514522
H	1.284764	0.881157	2.830917
H	2.155924	0.006982	1.568135
H	-0.938846	0.006741	1.860568
H	-0.895489	0.004633	-0.576608
H	0.956628	-0.002731	-0.557587
N	-0.310379	-0.980570	5.533636
C	-0.469666	-2.324984	6.108733
C	-0.477516	-2.355582	7.618097
C	0.437818	-2.973926	8.354985
H	0.562845	-0.575619	5.867129
H	-1.061839	-0.369114	5.838279
H	-1.404635	-2.744853	5.721169
H	0.351091	-2.944769	5.736136
H	-1.286689	-1.812264	8.106609
H	0.400707	-2.961066	9.439230
H	1.258877	-3.515628	7.893306

4IAIV

B	3.243503	1.064323	4.147531
H	2.979309	2.084348	4.708381
H	3.828182	1.086935	3.105110
H	2.921302	0.015455	4.621769
N	1.356402	1.139079	3.059464
C	1.228804	-0.010930	2.165873
C	0.010454	0.024596	1.275700
C	0.054829	0.054183	-0.051556
H	1.339029	2.011048	2.540395
H	0.610510	1.169778	3.746802
H	1.215895	-0.907077	2.795683
H	2.137279	-0.062646	1.558193
H	-0.954458	0.042779	1.782517
H	1.002668	0.038713	-0.583274
H	-0.847559	0.089169	-0.652867
N	5.158034	0.941648	5.187160
C	5.850469	-0.280998	4.825819
C	7.219413	-0.509655	5.425771
C	7.863088	0.309790	6.248786
H	5.680225	1.767592	4.914861
H	4.979324	0.995193	6.184408
H	5.930110	-0.307075	3.732067
H	5.198621	-1.122475	5.089426
H	7.692733	-1.446401	5.133844
H	7.435003	1.254633	6.569684
H	8.847167	0.063091	6.631393

4IBIV

B	3.353299	1.176101	3.984312
H	3.065697	2.143009	4.624151
H	3.152894	0.084921	4.428539
H	3.838880	1.298389	2.899737
N	1.381262	1.156014	3.057698
C	1.246867	-0.007116	2.182131
C	-0.002674	-0.010686	1.335381
C	-0.004019	-0.017828	0.007018
H	1.296663	2.021398	2.534219
H	0.679102	1.163270	3.790090
H	1.277088	-0.896035	2.821372
H	2.134032	-0.046145	1.542666
H	-0.949486	0.008870	1.875075
H	-0.927354	-0.014189	-0.562899
H	0.925151	-0.035893	-0.556427
N	5.330808	1.187211	4.903434
C	5.227081	0.959721	6.332612
C	6.504125	1.018821	7.140184
C	7.722173	1.252823	6.665846
H	5.900273	0.481988	4.447697
H	5.726989	2.097385	4.693749
H	4.753752	-0.018359	6.480379
H	4.514865	1.690751	6.734587
H	6.374582	0.850840	8.208701
H	8.584601	1.281308	7.322496
H	7.903641	1.425777	5.609309

4IHIV

B	2.682552	-1.263218	3.920708
H	3.606010	-1.317041	3.150692
H	2.698622	-0.256252	4.588990
H	2.582774	-2.257601	4.597081
N	1.339435	-1.186609	3.045530
C	1.250179	-0.000014	2.166424
C	-0.000101	0.000003	1.327977
C	0.000006	0.000586	0.000224
H	0.555933	-1.183652	3.717137
H	1.256434	-2.027385	2.477934
H	1.285921	0.873207	2.824570
H	2.146507	0.018719	1.542560
H	-0.945295	0.001493	1.869571
H	-0.924386	0.006401	-0.567410

H	0.928484	0.002345	-0.564337
N	-0.188424	-1.035429	5.568911
C	-0.350431	-2.358284	6.161906
C	-0.435981	-2.427163	7.671209
C	-0.348665	-1.396783	8.503378
H	-0.922484	-0.409190	5.885190
H	0.702025	-0.633931	5.856237
H	0.492657	-2.975623	5.828114
H	-1.252450	-2.819957	5.741593
H	-0.580336	-3.428483	8.074495
H	-0.420559	-1.533429	9.576604
H	-0.194732	-0.382762	8.147686

4IVHI

B	3.782887	0.109844	2.491263
H	4.743139	0.199744	1.766976
H	3.671100	1.053375	3.230276
H	3.755230	-0.943168	3.083733
N	2.499270	0.103859	1.525966
C	1.216064	-0.002857	2.231226
C	-0.000360	0.004892	1.342790
C	-0.004769	0.023778	0.015285
H	2.618939	-0.703471	0.893234
H	2.503863	0.948263	0.957591
H	1.164518	0.817347	2.954422
H	1.250022	-0.926238	2.819047
H	-0.947395	-0.010620	1.878556
H	0.909002	0.028636	-0.570853
H	-0.935908	0.028189	-0.539974
N	3.472604	-2.418473	0.346890
C	4.627093	-2.167984	-0.529569
C	5.661644	-3.267634	-0.517881
C	6.910156	-3.108771	-0.094401
H	3.802936	-2.549770	1.301289
H	2.990310	-3.269485	0.073924
H	4.247806	-2.021991	-1.547141
H	5.087739	-1.229015	-0.209329
H	5.329187	-4.245944	-0.865728
H	7.620132	-3.929280	-0.090626
H	7.263954	-2.146136	0.264651

4IVAIV

B	4.105846	0.004263	3.071496
H	4.928880	0.008382	2.207094
H	3.687363	1.035328	3.507774
H	3.695338	-1.031003	3.505404
N	2.512266	0.001380	1.582926
C	1.206691	-0.008283	2.215621
C	-0.003019	-0.010258	1.307805
C	0.017416	-0.004232	-0.019982
H	2.655194	-0.816483	0.999920
H	2.646811	0.826097	1.007620
H	1.162449	-0.883873	2.874728
H	1.153614	0.860488	2.883033
H	-0.961681	-0.017392	1.824870
H	-0.900853	-0.006288	-0.596684
H	0.948503	0.002894	-0.578388
N	5.670548	0.009338	4.590394
C	5.102385	0.004657	5.925328
C	6.068189	0.010045	7.089233
C	7.393381	0.017947	7.003934
H	6.246185	-0.808934	4.422194
H	6.238123	0.833713	4.424585
H	4.448054	-0.871933	6.005722
H	4.436534	0.872423	6.006991
H	5.598548	0.007100	8.072021
H	7.905605	0.021384	6.046643
H	8.014243	0.021484	7.892935

4IVBIV

B	4.108047	-0.119221	3.069316
H	3.677390	0.855001	3.610005
H	3.711163	-1.201193	3.383280
H	4.935239	-0.011267	2.214416
N	2.513612	-0.000409	1.580448
C	1.213183	-0.001912	2.223721
C	-0.004805	-0.007049	1.327538
C	0.000375	-0.004581	-0.000286
H	2.658477	0.832855	1.020252
H	2.639036	-0.809493	0.981440
H	1.167639	0.871103	2.885769
H	1.172952	-0.872946	2.889301
H	-0.957924	-0.013275	1.855001
H	-0.924029	-0.011039	-0.567087
H	0.924607	0.001694	-0.570400
N	5.703843	-0.241913	4.555245
C	6.460688	0.995227	4.595369
C	7.657900	1.047159	5.517665
C	8.083401	0.065435	6.303996
H	5.289200	-0.461928	5.454585
H	6.279971	-1.027556	4.272393
H	6.785863	1.218917	3.571884
H	5.767264	1.801829	4.862020
H	8.197420	1.993495	5.510214
H	8.956781	0.187635	6.934949
H	7.579126	-0.895400	6.346123

4IVHIV

B	3.778852	0.096625	2.497045
H	3.821610	-1.028686	2.937237
H	4.729875	0.351488	1.801382
H	3.600024	0.920578	3.356516
N	2.496222	0.135871	1.530187
C	1.215382	-0.038909	2.226744

C	0.001073	-0.016378	1.335762
C	-0.002831	0.061339	0.010257
H	2.619046	-0.632455	0.851683
H	2.485009	1.014236	1.016357
H	1.273171	-0.989457	2.768222
H	1.141464	0.741889	2.990301
H	-0.946832	-0.068807	1.867948
H	0.911577	0.106625	-0.573474
H	-0.934458	0.075646	-0.544208
N	3.204966	-2.431833	0.241250
C	4.582880	-2.321399	-0.229629
C	5.359343	-3.610500	-0.377905
C	4.909774	-4.830771	-0.110692
H	3.196955	-2.840924	1.172513
H	2.664874	-3.045150	-0.361698
H	5.115030	-1.659198	0.463582
H	4.577970	-1.803850	-1.196803
H	6.380699	-3.487177	-0.735313
H	5.540534	-5.703090	-0.239985
H	3.902606	-5.007115	0.254592

5IAI

B	1.184296	-0.003511	5.430371
H	0.616377	-1.053547	5.360128
H	0.552536	1.010832	5.386280
H	2.370585	0.031751	5.543437
N	0.945663	-0.038921	7.590405
C	-0.472284	-0.090971	7.931969
C	-0.757732	-0.116515	9.376762
C	-0.955648	-0.136036	10.557643
H	1.384196	0.790609	7.976933
H	1.439161	-0.847270	7.954900
H	-0.961088	0.775205	7.475821
H	-0.901296	-0.978249	7.456678
H	-1.135963	-0.153679	11.607484
N	1.355833	0.028891	3.263787
C	0.027311	-0.007330	2.660704
C	0.018258	0.011585	1.187912
C	0.045715	0.027894	-0.009172
H	1.857188	0.868540	2.992725
H	1.910819	-0.769388	2.972975
H	-0.539962	0.846693	3.042927
H	-0.481755	-0.906765	3.019999
H	0.065770	0.042318	-1.074246

5IBI

B	1.182826	0.091437	5.429453
H	2.370324	0.056691	5.547038
H	0.554626	-0.921889	5.367853
H	0.620592	1.144802	5.373455
N	0.992905	0.122715	7.602030
C	1.786687	1.224774	8.137348
C	1.741096	1.361204	9.603258
C	1.683420	1.442843	10.796606
H	1.310983	-0.767899	7.969975
H	0.013322	0.225925	7.846217
H	2.821580	1.081216	7.813281
H	1.438129	2.150811	7.670241
H	1.635528	1.519221	11.858129
N	1.357515	0.087931	3.255837
C	0.023733	-0.004944	2.669463
C	-0.002450	-0.009382	1.196768
C	0.011284	-0.012325	-0.000678
H	1.935117	-0.697104	2.973205
H	1.826911	0.938389	2.962114
H	-0.570345	0.833238	3.045931
H	-0.446697	-0.916900	3.048456
H	0.019199	-0.015769	-1.065992

5IHI

B	5.415413	-0.876862	2.164365
H	5.750792	-1.933867	2.632164
H	5.172353	-0.051284	3.013023
H	6.182889	-0.463816	1.333417
N	4.018995	-1.142941	1.417647
C	3.467542	0.062118	0.766270
C	2.137853	-0.163302	0.189720
C	1.054670	-0.366644	-0.275818
H	3.344797	-1.470564	2.128132
H	4.125653	-1.881468	0.725633
H	3.428260	0.847175	1.526141
H	4.174202	0.389342	-0.000567
H	0.090037	-0.536930	-0.695902
N	2.375701	-1.501665	3.844588
C	2.115822	-0.093869	4.167334
C	1.567000	0.135928	5.514312
C	1.118966	0.289563	6.613816
H	3.088468	-1.869557	4.468906
H	1.537539	-2.055868	3.989950
H	1.420173	0.309462	3.423746
H	3.059558	0.451566	4.061930
H	0.726742	0.432059	7.594208

5IAII

B	1.143260	0.044728	5.441570
H	2.321527	0.168589	5.582051
H	0.436747	1.010772	5.430910
H	0.662344	-1.037300	5.306355
N	1.343157	0.172588	3.262074
C	0.023967	0.001725	2.661675
C	0.010298	-0.011991	1.188740
C	0.028464	-0.021880	-0.008712
H	1.971790	-0.571814	2.978870
H	1.761886	1.054329	2.984759

H	-0.398908	-0.932568	3.042946
H	-0.620545	0.806480	3.027707
H	0.035422	-0.031744	-1.073981
N	0.867653	-0.045069	7.603144
C	-0.545624	-0.098709	7.983899
C	-1.087246	-1.451295	7.816934
C	-1.529305	-2.557959	7.714931
H	1.388857	-0.814515	8.010453
H	1.290258	0.825562	7.906092
H	-0.722015	0.214662	9.021597
H	-1.092727	0.589323	7.329751
H	-1.921217	-3.542420	7.605828

5IBII

B	1.194050	-0.155363	5.390750
H	2.374658	-0.278736	5.478057
H	0.700264	0.931742	5.349560
H	0.495206	-1.125978	5.338033
N	1.316880	-0.158800	3.205216
C	-0.014185	0.041473	2.642730
C	-0.069475	0.056781	1.170659
C	-0.080742	0.065931	-0.026814
H	1.714562	-1.042610	2.904738
H	1.951543	0.579962	2.920866
H	-0.664550	-0.750222	3.026902
H	-0.405402	0.985042	3.034683
H	-0.098550	0.077341	-1.091916
N	0.971591	-0.210855	7.560667
C	1.472791	-1.471629	8.113841
C	2.929311	-1.432338	8.278322
C	4.112877	-1.389009	8.445469
H	1.400746	0.588154	8.015176
H	-0.034213	-0.142238	7.670240
H	1.026506	-1.720980	9.085734
H	1.211567	-2.269890	7.410096
H	5.169516	-1.354252	8.575676

5IHII

B	0.610212	-1.167505	4.861088
H	1.325978	-2.072871	5.205514
H	-0.552833	-1.370179	5.120603
H	0.991347	-0.100392	5.267071
N	0.691655	-1.118610	3.258689
C	-0.079669	-0.003989	2.671908
C	0.028461	0.057461	1.210798
C	0.135806	0.101653	0.020250
H	0.308160	-2.010778	2.907138
H	1.661089	-1.055262	2.955889
H	-1.121073	-0.137044	2.976082
H	0.276211	0.925389	3.123560
H	0.226514	0.146777	-1.040600
N	-0.768058	-3.675668	3.050311
C	0.178593	-4.632194	3.641677
C	1.239191	-4.966609	2.683416
C	2.093498	-5.245814	1.893384
H	-1.266013	-4.098213	2.273604
H	-1.448063	-3.395248	3.751122
H	-0.298035	-5.563293	3.976139
H	0.626719	-4.153778	4.518516
H	2.859584	-5.495516	1.196454

5IIHI

B	-1.977950	-1.534327	3.274259
H	-2.402526	-0.640793	3.969820
H	-2.124562	-2.618635	3.782590
H	-2.390150	-1.482454	2.149271
N	-0.385626	-1.301025	3.225281
C	0.047762	-0.001947	2.658025
C	0.000418	-0.001060	1.195373
C	-0.000466	-0.000527	0.000152
H	-0.072232	-1.363291	4.205032
H	0.056609	-2.057008	2.706470
H	-0.625536	0.760846	3.058092
H	1.068196	0.225749	2.983156
H	-0.028895	0.002547	-1.065121
N	-0.471737	-1.504665	6.172011
C	0.236088	-1.278023	7.434145
C	-0.592086	-1.439026	8.642507
C	-1.294001	-1.576146	9.602504
H	-1.272948	-0.882135	6.092849
H	-0.868915	-2.440852	6.153529
H	0.655910	-0.267819	7.422676
H	1.082089	-1.969761	7.486763
H	-1.918206	-1.697115	10.457587

5IIAII

B	-2.469875	1.559633	3.335051
H	-2.348595	2.651373	3.800837
H	-2.493101	0.602683	4.047452
H	-2.566183	1.418148	2.154180
N	-4.658428	1.708451	3.405418
C	-5.270133	0.456736	2.953073
C	-5.357333	-0.512987	4.049566
C	-5.458066	-1.295229	4.949004
H	-4.820096	2.453204	2.736710
H	-5.026279	1.995842	4.306071
H	-4.636079	0.044470	2.159919
H	-6.277703	0.596080	2.539043
H	-5.530792	-1.997598	5.746470
N	-0.289541	1.316595	3.222058
C	0.060991	0.002099	2.679517
C	0.009113	0.005450	1.213835
C	0.001737	0.013575	0.017678
H	0.175796	2.061852	2.714749

H	-0.034452	1.383855	4.201163
H	1.060342	-0.336327	2.984476
H	-0.668430	-0.720627	3.062253
H	-0.022584	0.016818	-1.047215

5IIBII

B	-2.363717	1.727738	3.356388
H	-2.507209	1.535291	2.187306
H	-2.160230	2.828929	3.760769
H	-2.422564	0.807037	4.116904
N	-0.204918	1.340097	3.197283
C	0.053003	-0.001361	2.669569
C	0.008857	-0.006947	1.203825
C	0.005676	-0.001275	0.007662
H	0.293074	2.048622	2.669078
H	0.071768	1.408299	4.170307
H	-0.728772	-0.666057	3.054393
H	1.023523	-0.408593	2.983093
H	-0.011823	0.002314	-1.057309
N	-4.538948	2.032748	3.482866
C	-4.924400	3.229085	2.730116
C	-4.762830	4.437752	3.544484
C	-4.665272	5.422308	4.216752
H	-4.904528	2.057949	4.428722
H	-4.878777	1.193245	3.026857
H	-4.269147	3.296939	1.854216
H	-5.961919	3.195230	2.371771
H	-4.557602	6.299893	4.810667

5IIHII

B	-2.145848	-1.082064	3.281894
H	-2.548289	-2.100197	3.789781
H	-2.360293	-0.109418	3.968670
H	-2.521588	-0.940303	2.150586
N	-0.542827	-1.223880	3.260378
C	0.189916	-0.080412	2.668084
C	0.241220	-0.170383	1.208178
C	0.312573	-0.257694	0.017911
H	-0.264739	-1.329101	4.245706
H	-0.274728	-2.079986	2.779962
H	1.208021	-0.043244	3.069090
H	0.348489	-0.327960	-1.044620
H	-0.332455	0.828740	2.976749
N	0.271721	-1.532031	6.146446
C	-0.358677	-0.292672	6.631776
C	0.384525	0.874291	6.142420
C	1.014566	1.813767	5.752171
H	-0.227122	-2.337899	6.511634
H	1.232277	-1.591205	6.469273
H	-0.418507	-0.234572	7.726483
H	-1.379490	-0.255240	6.234566
H	1.563203	2.659443	5.406250

6A

C	-0.053591	2.307562	0.000000
Al	0.004501	0.306420	0.000000
N	2.225404	0.319593	0.000000
C	2.867694	-1.001092	0.000000
H	3.961503	-0.949567	0.000000
C	0.011613	-0.662496	-1.754877
N	-2.218380	0.292257	0.000000
C	-2.841598	-1.037495	0.000000
H	-3.936061	-1.001712	0.000000
C	0.011613	-0.662496	1.754877
H	-2.502985	-1.581410	0.883288
H	-2.511017	0.824661	-0.814643
H	-2.511017	0.824661	0.814643
H	-2.502985	-1.581410	-0.883288
H	0.882861	-0.415088	-2.377141
H	0.020517	-1.756266	-1.646837
H	-0.864567	-0.428942	-2.375543
H	0.925639	2.804372	0.000000
H	-0.585210	2.700804	-0.878383
H	-0.585210	2.700804	0.878383
H	0.882861	-0.415088	2.377141
H	-0.864567	-0.428942	2.375543
H	0.020517	-1.756266	1.646837
H	2.510267	0.856141	-0.814779
H	2.510267	0.856141	0.814779
H	2.536820	-1.549657	0.883332
H	2.536820	-1.549657	-0.883332

6B

C	0.005126	0.008784	0.007807
Al	0.001579	-0.000859	2.008866
N	2.222154	-0.005460	1.995499
C	2.902212	-0.145957	3.289044
C	-0.046442	1.749605	2.985263
C	0.009916	-1.722292	3.032802
N	-2.228194	0.042535	2.023318
C	-2.924226	-0.965230	1.213968
H	-0.943131	-2.265597	3.030230
H	0.254406	-1.557582	4.091536
H	0.757375	-2.435161	2.657122
H	-0.174974	-0.988981	-0.416206
H	0.946501	0.358083	-0.437534
H	-0.776250	0.660451	-0.407533
H	-0.615132	2.505812	2.424906
H	-0.536670	1.666809	3.965782
H	0.932577	2.205788	3.180693
H	-2.490984	-0.037833	3.001871
H	-2.494543	0.978290	1.729892
H	-2.587371	-1.957107	1.519017
H	-2.648969	-0.822657	0.168142

H	-4.014216	-0.915979	1.307184
H	2.481343	0.869479	1.547965
H	2.503230	-0.747606	1.360469
H	2.630657	-1.108841	3.722850
H	2.547003	0.639590	3.958524
H	3.992512	-0.081927	3.211262

6H

Al	0.002174	-0.024386	1.999867
C	1.780995	-0.010468	2.873609
C	0.028529	-0.050624	0.020086
C	-1.390483	1.093052	2.843792
H	1.755927	-0.270596	3.939833
H	2.510985	-0.677981	2.396818
H	2.218587	0.995364	2.821385
H	-1.375992	1.049433	3.940273
H	-2.406884	0.825476	2.524824
H	-1.258803	2.150180	2.579345
H	0.633799	-0.862263	-0.406346
H	0.448047	0.881000	-0.381104
H	-0.973788	-0.144397	-0.418447
N	-0.655636	-1.916152	2.386179
C	-0.905370	-2.227939	3.804558
H	0.073437	-2.541425	2.009513
H	-1.498983	-2.078183	1.840763
H	0.020363	-2.079194	4.362788
H	-1.244349	-3.257905	3.946648
H	-1.657308	-1.543494	4.200490
N	1.844023	-3.235268	1.335157
C	2.101342	-4.525320	0.690344
H	2.485159	-3.084937	2.108208
H	2.006782	-2.468705	0.687454
H	1.413882	-4.650496	-0.148911
H	3.125113	-4.641784	0.314237
H	1.904169	-5.329434	1.402872

7IAI

Al	-0.001869	0.000127	2.017312
C	-0.025644	1.757157	2.981423
C	-0.025513	-1.756730	2.981746
C	0.002135	-0.000149	0.015281
H	0.854052	2.377799	2.761852
H	-0.053202	1.649707	4.074923
H	-0.893746	2.376823	2.717476
H	0.853947	-2.377513	2.761597
H	-0.052220	-1.649106	4.075249
H	-0.893897	-2.376326	2.718572
H	-0.516142	-0.879241	-0.393680
H	-0.517938	0.877685	-0.394083
H	0.996747	0.000761	-0.449829
N	2.223992	0.000092	2.073814
C	2.840946	-0.000406	3.406568
C	4.373883	-0.000308	3.403669
C	4.944799	-0.000797	4.827225
H	2.525525	-0.814519	1.544125
H	2.525466	0.815102	1.544705
H	2.465686	-0.879517	3.939119
H	2.465570	0.878211	3.939843
H	4.734723	-0.880263	2.857507
H	4.734607	0.880105	2.858166
H	4.613160	-0.884951	5.380029
H	4.613043	0.882898	5.380689
H	6.037508	-0.000724	4.817513
N	-2.231255	0.000070	1.961632
C	-2.911846	-0.000022	3.263038
C	-4.442892	-0.000293	3.186599
C	-5.081202	-0.000329	4.581281
H	-2.506827	-0.814619	1.418260
H	-2.506974	0.814705	1.418254
H	-2.563117	0.878878	3.813657
H	-2.562803	-0.878777	3.813701
H	-4.776974	-0.880550	2.624159
H	-4.777276	0.879793	2.624073
H	-4.776412	0.883644	5.149627
H	-4.776168	-0.884177	5.149691
H	-6.172197	-0.000478	4.519390

7IBI

Al	0.008076	0.002854	2.012953
C	-0.001261	-0.008505	0.012615
C	-1.736963	0.020007	3.002303
C	1.728309	0.001384	3.034911
H	1.002318	0.143476	-0.408638
H	-0.373763	-0.943809	-0.426374
H	-0.631406	0.786886	-0.408700
H	-1.591380	0.088610	4.090019
H	-2.344617	-0.879833	2.836645
H	-2.387287	0.863585	2.732939
H	1.554344	-0.121178	4.113545
H	2.400405	-0.817299	2.742584
H	2.319890	0.919189	2.929341
N	-0.035202	2.242216	2.020199
C	0.974917	2.964805	1.237024
C	0.849256	4.492174	1.283790
C	1.940460	5.179118	0.452898
H	0.011459	2.517789	2.998944
H	-0.969335	2.486576	1.700299
H	1.958390	2.658119	1.605239
H	0.900468	2.612061	0.204231
H	0.906654	4.829054	2.325933
H	-0.139952	4.784737	0.911546
H	2.935695	4.925200	0.830145
H	1.837684	6.266669	0.481595
H	1.890071	4.864902	-0.594048
N	0.012307	-2.227710	2.022860

C	0.068696	-2.888639	3.332993
C	0.055375	-4.420856	3.279184
C	0.123571	-5.040382	4.680720
H	0.800553	-2.515276	1.447171
H	-0.826573	-2.508880	1.520591
H	-0.781313	-2.525468	3.919132
H	0.974227	-2.537798	3.836159
H	0.904320	-4.767752	2.677717
H	-0.853533	-4.758543	2.766777
H	-0.730629	-4.725937	5.287855
H	0.118627	-6.132188	4.634915
H	1.035011	-4.729306	5.200061

7IHI

Al	-0.004235	0.019329	1.993138
C	1.800311	0.014831	2.808782
C	-0.021492	0.011958	0.009964
C	-1.381648	-1.093357	2.866966
H	1.781264	-0.048207	3.904127
H	2.385815	-0.846684	2.462286
H	2.393532	0.905615	2.556691
H	-0.918956	0.472892	-0.424795
H	0.845558	0.512333	-0.441520
H	-0.001475	-1.019193	-0.366805
H	-1.164394	-2.160428	2.727481
H	-2.388968	-0.933091	2.460416
H	-1.444177	-0.937153	3.951713
N	-0.643212	1.909575	2.401509
C	-0.554165	2.322652	3.815242
C	-1.044728	3.751072	4.066798
C	-0.917032	4.144821	5.543336
H	-0.065185	2.538185	1.821636
H	-1.604014	2.005318	2.077508
H	0.493230	2.224659	4.115596
H	-1.128548	1.609421	4.414946
H	-2.090693	3.836223	3.748067
H	-0.465493	4.440506	3.441839
H	0.123862	4.085314	5.875221
H	-1.265330	5.166712	5.711406
H	-1.509013	3.479503	6.178995
N	1.396942	3.271061	0.643047
C	0.939703	3.609973	-0.708038
C	2.053876	3.772262	-1.750844
C	1.499576	4.104121	-3.141938
H	1.913394	2.393988	0.624597
H	2.040678	3.977967	0.986833
H	0.250737	2.822222	-1.031302
H	0.357677	4.536457	-0.646467
H	2.637859	2.845222	-1.792858
H	2.738893	4.563919	-1.423161
H	0.919328	5.031952	-3.122338
H	2.305141	4.228039	-3.870020
H	0.843318	3.305279	-3.500074

8IAI

C	-0.001853	-0.000899	0.000478
Al	0.000074	-0.000050	2.006211
C	1.758840	0.003611	2.936840
C	-1.752867	0.040951	2.947038
N	0.016337	-2.305333	1.907310
C	0.022872	-3.273938	2.990601
C	-1.140375	-3.286738	3.962504
C	0.231696	-2.797369	4.417160
N	-0.024430	2.301789	1.790298
C	-0.008381	3.325344	2.821462
C	1.166339	3.380374	3.777407
C	-0.202738	2.922307	4.272593
H	-0.916153	2.327562	1.301859
H	0.685686	2.503051	1.089801
H	-0.427074	4.285025	2.528015
H	-2.464726	-0.664032	2.497360
H	-1.674830	-0.234544	4.007599
H	-2.240800	1.023644	2.927689
H	-0.074604	-0.988609	-0.472971
H	-0.841239	0.578838	-0.409409
H	0.911746	0.455005	-0.406641
H	2.245683	-0.979381	2.963589
H	2.467150	0.683855	2.445430
H	1.689889	0.333310	3.982402
H	1.524978	4.358965	4.073829
H	1.928544	2.619138	3.668550
H	-0.773835	3.585870	4.911133
H	-0.323883	1.865526	4.475592
H	-0.715259	-2.537393	1.239526
H	0.893506	-2.360200	1.395062
H	0.443799	-4.244865	2.740963
H	0.814399	-3.425225	5.080835
H	0.348904	-1.731285	4.566092
H	-1.490844	-4.250628	4.312024
H	-1.907549	-2.535142	3.824161

8IBI

C	0.015236	0.003850	0.003268
Al	-0.004604	0.000112	1.997639
C	1.688990	-0.004513	3.043625
N	-0.118385	-2.298572	2.160639
C	0.737805	-3.328502	1.599917
C	2.058457	-2.936757	0.963193
C	0.897876	-3.411213	0.093446
C	-1.772921	-0.041986	2.930728
N	-0.100509	2.303439	1.881850
C	-0.118042	3.296512	2.941237
C	1.058106	3.362349	3.895977
C	-0.294030	2.846582	4.380490
H	-0.995058	2.307010	1.397439

H	0.598053	2.550585	1.184811
H	-0.569914	4.249349	2.675818
H	-2.528736	-0.599127	2.358846
H	-1.723279	-0.523805	3.918475
H	-2.201281	0.951188	3.113230
H	-0.767167	-0.652019	-0.400575
H	-0.152935	0.984456	-0.462070
H	0.966289	-0.362193	-0.405575
H	2.142290	-0.998961	3.135333
H	2.457679	0.636483	2.591074
H	1.547616	0.362563	4.068953
H	1.386794	4.343100	4.218937
H	1.841881	2.627082	3.762184
H	-0.884880	3.473096	5.038351
H	-0.381740	1.780603	4.549841
H	-0.021582	-2.293660	3.173439
H	-1.094373	-2.514691	1.971353
H	0.722705	-4.279988	2.126528
H	0.950501	-4.398404	-0.350371
H	0.394345	-2.658912	-0.501328
H	2.906398	-3.595831	1.107957
H	2.290953	-1.879472	0.931065

8IHI

Al	-0.005930	-0.009488	1.994443
C	-1.389717	1.125143	2.856664
C	1.787561	0.004720	2.818881
C	-0.018687	-0.009720	0.013521
H	-1.776788	1.897259	2.178526
H	-1.005079	1.658044	3.735437
H	-2.257582	0.548956	3.205899
H	1.778801	-0.026382	3.915305
H	2.308432	0.931520	2.542916
H	2.430198	-0.815942	2.474470
H	0.391142	0.933722	-0.370981
H	-1.016973	-0.111172	-0.432384
H	0.603399	-0.804007	-0.421733
N	-0.783163	-1.899295	2.251262
C	-0.906490	-2.592731	3.528733
C	0.324678	-2.782542	4.391727
C	-0.777554	-1.820620	4.828382
H	-0.288211	-2.499937	1.593068
H	-1.725597	-1.755337	1.852280
H	-1.620828	-3.410817	3.520090
H	1.248678	-2.337521	4.042247
H	0.429389	-3.724676	4.916393
H	-0.565417	-0.760061	4.764368
H	-1.424265	-2.110264	5.647928
N	-3.448148	-0.994799	1.075457
C	-4.043003	-1.491437	-0.141796
C	-3.133124	-2.228802	-1.106493
C	-4.169534	-2.997440	-0.289560
H	-3.026798	-0.079839	0.929460
H	-4.150468	-0.882662	1.801080
H	-4.835494	-0.894562	-0.589719
H	-2.091713	-2.323685	-0.821318
H	-3.306284	-2.103926	-2.168564
H	-5.038500	-3.391735	-0.802601
H	-3.808798	-3.600531	0.535602

8IAII

C	-0.009939	0.004866	0.015857
Al	-0.008726	-0.001143	2.019316
N	2.299364	0.000515	1.811228
C	3.321176	-0.002739	2.843229
C	3.327833	1.116107	3.867013
C	2.920114	-0.296188	4.277536
C	0.052638	-1.760836	2.958017
C	-0.032596	1.755177	2.962720
N	-2.241216	-0.079861	2.048223
C	-2.879989	-0.048888	3.348915
C	-4.365417	-0.341211	3.516891
C	-3.309919	-1.344873	3.990097
H	2.492508	0.733049	1.131900
H	2.332885	-0.876589	1.297300
H	4.297164	-0.366604	2.530360
H	-1.001888	2.268088	2.902795
H	0.203391	1.674837	4.032764
H	0.699077	2.453832	2.536990
H	-1.009695	-0.027759	-0.437280
H	0.471372	0.902685	-0.396661
H	0.529453	-0.854667	-0.407090
H	-0.640867	-2.477777	2.496304
H	1.037369	-2.243687	2.957986
H	-0.250892	-1.685384	4.011100
H	3.602415	-0.876814	4.887190
H	1.867180	-0.472940	4.459662
H	4.291785	1.491406	4.189684
H	2.540051	1.855419	3.798711
H	-2.540890	0.714718	1.487161
H	-2.506032	-0.917692	1.536088
H	-2.443056	0.703359	3.996130
H	-4.919679	0.217584	4.262038
H	-4.928001	-0.595703	2.624864
H	-3.148798	-1.467209	5.054175
H	-3.185625	-2.253705	3.410837

8IBII

Al	-0.002251	-0.003049	1.993706
C	0.165280	1.751574	2.951548
C	-0.166425	-1.688744	3.035767
C	-0.003968	-0.002005	-0.007062
H	0.900212	2.420788	2.482020
H	-0.765555	2.331125	2.999978
H	0.492479	1.625552	3.993670

H	-1.181189	-1.849144	3.419180
H	0.082353	-2.576263	2.438672
H	0.496190	-1.705164	3.910890
H	0.990693	0.030546	-0.468206
H	-0.490459	-0.901343	-0.412732
H	-0.557052	0.853887	-0.419750
N	2.295688	0.001559	2.031850
C	2.729811	-2.160454	0.723438
C	3.160747	-2.398291	2.168097
C	3.234404	-1.006509	1.571591
H	2.378706	0.832222	1.450857
H	2.532790	0.293893	2.977290
H	4.231564	-0.639526	1.340292
H	3.370280	-2.517663	-0.074289
H	1.667414	-2.188394	0.513775
H	4.096121	-2.913479	2.351647
H	2.373412	-2.586019	2.887422
N	-2.237749	0.255389	1.880494
C	-3.836397	-0.828333	3.554560
C	-4.456793	0.524772	3.199693
C	-2.948864	0.321962	3.141505
H	-2.610650	-0.480678	1.287183
H	-2.334206	1.127302	1.365779
H	-2.355936	0.791562	3.919123
H	-3.966943	-1.638695	2.844697
H	-3.822381	-1.140644	4.591672
H	-4.861821	1.132150	4.000801
H	-4.988480	0.596893	2.256936

8IHII

Al	-0.011903	0.004519	1.992883
C	-0.570401	-1.694244	2.852328
C	-0.690988	1.664703	2.814745
C	0.001164	-0.011004	0.010885
H	-1.271524	-2.257525	2.222713
H	-1.083122	-1.530528	3.808685
H	0.267965	-2.370045	3.068743
H	-0.628728	1.679288	3.909844
H	-1.755314	1.783370	2.570376
H	-0.193754	2.571855	2.447708
H	-1.013361	-0.135836	-0.389059
H	0.605230	-0.818569	-0.425001
H	0.381535	0.926648	-0.416220
N	2.034196	-0.011344	2.233312
C	2.744580	0.122160	3.499719
C	2.468284	1.318983	4.387598
C	2.005146	-0.073266	4.809522
H	2.396811	0.676159	1.573878
H	2.251474	-0.936328	1.825553
H	3.772136	-0.228628	3.466863
H	1.699971	2.010297	4.062777
H	3.310323	1.765295	4.903045
H	0.942564	-0.278149	4.760011
H	2.532019	-0.575818	5.611986
N	2.273784	-2.825065	1.102094
C	3.179083	-3.238379	0.055634
C	2.792702	-3.009995	-1.388011
C	2.897196	-4.437626	-0.842939
H	1.313152	-2.798129	0.768451
H	2.292172	-3.482541	1.877140
H	4.219352	-3.063427	0.311581
H	1.798214	-2.620919	-1.581692
H	3.552788	-2.661408	-2.076944
H	1.967827	-4.972025	-0.677754
H	3.729352	-5.052706	-1.166095

8IIHI

Al	0.000192	0.000126	1.973604
C	-0.602158	1.667366	2.858756
C	-0.563241	-1.699844	2.820065
C	0.000173	0.000552	0.000823
H	-0.261822	2.569856	2.334795
H	-1.698147	1.725185	2.881620
H	-0.272837	1.767927	3.902357
H	0.008647	-2.561863	2.449094
H	-1.613328	-1.914232	2.581085
H	-0.489498	-1.721919	3.914840
H	0.577386	-0.829646	-0.428087
H	-1.019592	-0.106721	-0.391368
H	0.400414	0.927209	-0.428613
N	1.993890	0.000776	2.445213
C	2.725448	1.200652	2.066587
C	3.293249	1.305638	0.673246
C	4.232517	1.171738	1.878019
H	2.426470	-0.818642	2.022272
H	2.035517	-0.123129	3.468871
H	2.282213	2.089875	2.500192
H	3.176807	0.443983	0.024257
H	3.231948	2.260828	0.166532
H	4.734378	0.219757	2.015216
H	4.808426	2.036905	2.184875
N	1.497866	-0.059965	5.452324
C	1.731428	-1.173245	6.340698
C	1.875013	-2.543901	5.706950
C	3.097567	-1.833991	6.284387
H	0.507821	0.025183	5.233266
H	1.785175	0.812576	5.886237
H	1.250466	-1.140786	7.316631
H	1.476830	-3.397990	6.241307
H	1.779130	-2.593959	4.628456
H	3.522331	-2.210592	7.207206
H	3.812918	-1.417564	5.584693

8IIAII

C	0.000000	0.000000	0.000000

Al	0.000000	0.000000	2.004896
N	2.246284	0.000000	2.003210
C	2.922600	-0.020730	3.283893
C	3.390928	1.279112	3.887069
C	4.417203	0.250964	3.399346
N	-2.250630	-0.039248	1.893900
C	-2.981445	-0.148911	3.139815
C	-4.498987	-0.029264	3.188410
C	-3.607383	1.086001	3.741675
C	0.012759	1.725448	2.999300
C	-0.009244	-1.763396	2.951321
H	-2.450418	-0.834694	1.291588
H	-2.528513	0.794044	1.381865
H	-2.516700	-0.851596	3.822594
H	0.872874	-2.376743	2.721317
H	-0.028043	-1.660775	4.045532
H	-0.875623	-2.386877	2.691207
H	0.986491	0.120323	-0.467139
H	-0.408605	-0.935663	-0.408264
H	-0.620330	0.808340	-0.412482
H	0.616954	2.484135	2.481415
H	-0.976247	2.172880	3.153098
H	0.459887	1.611760	3.995738
H	-5.044443	-0.652016	3.887929
H	-5.012921	0.165828	2.253067
H	-3.546085	1.221661	4.814424
H	-3.547457	2.005713	3.169098
H	2.497289	-0.820806	1.456336
H	2.527847	0.811483	1.458732
H	2.495016	-0.756902	3.955889
H	4.988543	-0.300402	4.137078
H	4.953494	0.480359	2.484539
H	3.266257	1.424199	4.953164
H	3.258117	2.177885	3.293927

8IIBII

Al	0.000000	0.000000	2.003030
C	0.000000	0.000000	0.000000
C	1.743747	0.000000	2.981855
C	-1.730109	-0.002691	2.996560
H	0.622178	0.802515	-0.420052
H	0.377084	-0.928361	-0.450116
H	-1.007683	0.146195	-0.413669
H	2.198348	0.986396	3.145192
H	1.645026	-0.456099	3.975779
H	2.502815	-0.592591	2.451452
H	-1.598325	0.256864	4.057004
H	-2.263602	-0.962017	2.984481
H	-2.431756	0.734347	2.586105
N	0.047040	-2.250528	1.976861
C	1.314573	-3.376127	3.878960
C	0.317334	-4.423479	3.371829
C	0.015047	-2.935766	3.252425
H	-0.751822	-2.517862	1.405568
H	0.880711	-2.503500	1.452540
H	-0.739132	-2.525528	3.914629
H	1.435897	-3.248965	4.947778
H	2.221542	-3.224793	3.303134
H	-0.236023	-5.006019	4.099166
H	0.575366	-4.954612	2.461592
N	0.028692	2.252519	2.013920
C	-2.191123	3.506610	1.927409
C	-1.142966	4.480575	1.383344
C	-0.958361	2.974995	1.238024
H	-0.012699	2.522901	2.993832
H	0.967768	2.474111	1.690846
H	-1.085166	2.550422	0.248403
H	-2.250886	3.383607	3.003858
H	-3.141290	3.424205	1.413677
H	-0.518139	4.991857	2.108219
H	-1.383634	5.059971	0.499565

8IIHII

Al	0.021312	-0.004489	1.999508
C	-0.514187	-1.700864	2.880775
C	-0.596330	1.643677	2.903964
C	-0.001157	-0.014453	0.026016
H	0.245667	-2.491676	2.808679
H	-0.755686	-1.576716	3.944518
H	-1.418151	-2.113458	2.414604
H	-0.310831	2.563203	2.377680
H	-1.691340	1.661134	2.979601
H	-0.221787	1.737878	3.933287
H	0.425799	0.900533	-0.403786
H	0.553752	-0.860210	-0.402420
H	-1.023182	-0.093151	-0.366309
N	2.028660	0.029258	2.409957
C	2.706433	1.277157	2.092939
C	3.244729	1.482969	0.698355
C	4.209359	1.319793	1.878909
H	2.467421	-0.739263	1.905526
H	2.118185	-0.183903	3.416703
H	2.238685	2.123668	2.582264
H	3.137816	2.460637	0.244545
H	3.152488	0.652851	0.005783
H	4.753004	0.383796	1.953897
H	4.754641	2.189383	2.226422
N	1.634507	-0.612158	5.333599
C	2.517585	-0.710896	6.471071
C	3.075400	-2.062589	6.852223
C	2.087413	-1.353323	7.785226
H	1.144140	-1.487582	5.170138
H	0.914808	0.089881	5.490680
H	3.196181	0.132637	6.547035
H	2.707259	-2.923168	6.303035
H	4.114354	-2.131953	7.151687

H	2.464072	-0.940705	8.714225
H	1.079867	-1.751977	7.835324

9IAI

Al	-0.002632	-0.001938	2.018418
C	-0.022666	1.747311	2.998423
C	0.001691	-0.000270	0.017275
C	-0.034745	-1.753824	2.991009
H	-0.888095	2.370870	2.735128
H	-0.054444	1.629621	4.090758
H	0.859742	2.367214	2.787472
H	-0.455022	0.912184	-0.391683
H	0.993867	-0.071167	-0.447528
H	-0.576856	-0.840315	-0.392722
H	0.842001	-2.378966	2.772594
H	-0.061317	-1.640364	4.083953
H	-0.905974	-2.370634	2.730527
N	2.215127	-0.006446	2.073309
C	2.819615	-0.002709	3.417005
C	4.323913	-0.101766	3.404977
C	5.009742	-1.085562	3.974996
H	2.526181	-0.825002	1.554970
H	2.518465	0.806018	1.541312
H	2.388074	-0.837472	3.974992
H	2.498019	0.920871	3.908443
H	4.854806	0.693783	2.882053
H	6.093581	-1.119088	3.942316
H	4.506574	-1.890371	4.504299
N	-2.228821	0.008063	1.962039
C	-2.895521	0.004448	3.275883
C	-4.397507	0.105791	3.193864
C	-5.108363	1.087918	3.735447
H	-2.509514	-0.803166	1.416190
H	-2.513720	0.827640	1.430535
H	-2.599164	-0.920314	3.780902
H	-2.489396	0.837656	3.854786
H	-4.904217	-0.686837	2.643241
H	-6.189454	1.122825	3.652249
H	-4.629741	1.889869	4.291186

9IBI

Al	-0.004365	0.008644	2.013327
C	-0.010369	0.007855	0.013559
C	-0.039129	1.723320	3.045212
C	0.041099	-1.744698	2.985481
H	-0.922561	-0.415519	-0.428125
H	0.819182	-0.573572	-0.411788
H	0.083627	1.020771	-0.402820
H	0.897722	2.293502	3.014920
H	-0.819726	2.413718	2.696567
H	-0.243819	1.544219	4.110335
H	0.116166	-1.612659	4.074264
H	0.892209	-2.378530	2.700985
H	-0.850047	-2.365070	2.817808
N	2.236736	0.007907	2.031699
C	2.932860	1.030651	1.231511
C	4.433072	0.987503	1.374597
C	5.172323	1.993222	1.827476
H	2.508152	-0.923881	1.727573
H	2.516506	0.083522	3.007567
H	2.641880	0.871690	0.188950
H	2.550353	2.009785	1.530280
H	4.914540	0.052866	1.086686
H	4.722072	2.937845	2.120714
H	6.250788	1.913641	1.913622
N	-2.228980	-0.035917	2.010941
C	-2.898878	0.025333	3.322396
C	-4.400723	-0.075862	3.236151
C	-5.237835	0.869824	3.645918
H	-2.467823	-0.901396	1.532019
H	-2.561706	0.720462	1.416994
H	-2.491636	-0.792413	3.926283
H	-2.606507	0.962789	3.800470
H	-4.795383	-0.992926	2.798648
H	-6.313243	0.755880	3.558922
H	-4.873648	1.793328	4.088112

9IHI

Al	0.015964	-0.000452	1.988548
C	-0.590166	-1.665390	2.858793
C	0.012350	-0.014603	0.007673
C	-0.538276	1.707929	2.821706
H	-0.388554	-1.698069	3.937324
H	-0.133730	-2.562342	2.419710
H	-1.675049	-1.793393	2.751077
H	0.718576	-0.735901	-0.426003
H	-0.978815	-0.305749	-0.364812
H	0.227163	0.961614	-0.446096
H	-1.547138	1.991731	2.494953
H	-0.573951	1.662604	3.917564
H	0.112849	2.555065	2.563407
N	2.023711	-0.007873	2.392625
C	2.385314	0.250290	3.804627
C	3.867168	0.139097	4.051606
C	4.416493	-0.705039	4.916308
H	2.432217	0.728354	1.797333
H	2.424446	-0.896901	2.099389
H	2.029952	1.258311	4.039568
H	1.835777	-0.450719	4.438162
H	4.498543	0.803854	3.462944
H	5.490595	-0.750546	5.061392
H	3.808633	-1.377719	5.515379
N	2.572911	2.387624	0.639288
C	2.999357	2.047327	-0.727207
C	2.511766	3.009357	-1.783267

C	1.694705	2.668120	-2.773122
H	2.990600	3.264771	0.935748
H	1.564336	2.527589	0.655704
H	4.093966	2.006051	-0.729750
H	2.632933	1.042796	-0.958361
H	2.848605	4.041720	-1.689060
H	1.351812	3.390915	-3.505944
H	1.338029	1.646885	-2.879154

9IAIV

Al	0.002328	0.004909	2.014498
C	1.750810	0.000062	2.991977
C	-1.746226	0.108780	2.988271
C	0.007393	-0.000483	0.013780
H	2.353440	-0.898258	2.800213
H	1.632880	0.057846	4.083296
H	2.391469	0.847855	2.712642
H	-1.625694	0.165472	4.079476
H	-2.399372	-0.754925	2.801683
H	-2.337901	0.989706	2.703401
H	-0.880258	0.503563	-0.394670
H	0.875624	0.538652	-0.391213
H	0.028917	-0.991307	-0.458850
N	-0.074449	-2.195408	2.066552
C	-0.106531	-2.820636	3.401468
C	-0.125247	-4.327596	3.359563
C	0.826262	-5.099274	3.871892
H	-0.897973	-2.460942	1.530785
H	0.729615	-2.537649	1.544888
H	-0.996589	-2.437550	3.910268
H	0.767135	-2.467475	3.954969
H	-0.981777	-4.785675	2.864906
H	0.774587	-6.181410	3.814461
H	1.691120	-4.671137	4.371698
N	0.074645	2.247252	1.926646
C	0.067612	2.924056	3.221989
C	0.132108	4.432445	3.192923
C	0.206559	5.192885	2.107105
H	-0.716045	2.548758	1.362287
H	0.914762	2.484649	1.404713
H	-0.836322	2.608154	3.754445
H	0.911151	2.534235	3.802886
H	0.113057	4.904764	4.173760
H	0.229074	4.771850	1.106569
H	0.248302	6.273762	2.181686

9IBIV

Al	0.000050	-0.002514	2.011113
C	0.018490	-1.721636	3.039072
C	0.006407	-0.001059	0.011735
C	-0.053866	1.745765	2.981111
H	0.263996	-1.552557	4.097062
H	0.766735	-2.433953	2.664119
H	-0.934467	-2.266563	3.039167
H	0.959961	0.312564	-0.433674
H	-0.211694	-0.991732	-0.410888
H	-0.748727	0.681836	-0.401716
H	-0.697623	2.475263	2.469375
H	-0.456166	1.647007	3.999529
H	0.918747	2.242270	3.091362
N	2.234696	-0.007624	2.004568
C	2.917868	-0.070896	3.308747
C	4.418873	0.029578	3.208640
C	5.140953	1.004623	3.748450
H	2.517962	0.834152	1.507893
H	2.511603	-0.792320	1.418940
H	2.626107	-1.015413	3.776840
H	2.523803	0.737717	3.929844
H	4.916870	-0.758753	2.644190
H	6.220609	1.036072	3.647530
H	4.673247	1.803546	4.317711
N	-2.236323	0.008115	2.047343
C	-2.923391	-0.950585	1.183727
C	-4.426636	-1.012300	1.313664
C	-5.173389	-0.285679	2.136380
H	-2.472998	-0.162426	3.022328
H	-2.537683	0.956270	1.836516
H	-2.501905	-1.942685	1.382859
H	-2.655439	-0.715210	0.148426
H	-4.907393	-1.732371	0.653426
H	-6.251711	-0.396649	2.161353
H	-4.744800	0.446097	2.814370

9IHIV

Al	-0.004513	0.010551	1.993818
C	1.784933	0.001675	2.840396
C	-1.409138	-1.073670	2.861099
C	-0.010365	0.007540	0.011709
H	2.396927	0.879730	2.589936
H	1.743121	-0.046957	3.935986
H	2.364924	-0.873308	2.519179
H	-2.420127	-0.818599	2.516374
H	-1.412431	-0.989673	3.955407
H	-1.273519	-2.140155	2.639516
H	-0.922981	0.439288	-0.421925
H	0.839321	0.529782	-0.448144
H	0.036141	-1.023849	-0.362494
N	-0.626794	1.921164	2.389265
C	-0.588061	2.313427	3.815924
C	-1.150993	3.689989	4.055012
C	-2.196497	3.938282	4.834766
H	-1.572631	2.044965	2.032996
H	-0.006884	2.536149	1.840425
H	0.459885	2.264437	4.127723
H	-1.140631	1.567538	4.393529

H	-0.651658	4.508244	3.537541
H	-2.571917	4.945928	4.977960
H	-2.710589	3.138479	5.360975
N	1.554973	3.155518	0.707263
C	1.109231	3.531744	-0.629993
C	2.152291	3.537934	-1.725796
C	3.434473	3.226188	-1.582142
H	1.971478	2.226685	0.689933
H	2.274222	3.792958	1.036078
H	0.303352	2.847159	-0.922340
H	0.654055	4.527934	-0.572316
H	1.779646	3.823710	-2.708331
H	3.851236	2.928996	-0.624743
H	4.115020	3.248984	-2.425885

9IVHI

Al	0.000108	-0.000321	1.982579
C	-0.564878	-1.694882	2.836204
C	-0.598349	1.674123	2.840931
C	-0.000074	0.001368	-0.000171
H	-1.586454	-1.962606	2.536746
H	0.064653	-2.553718	2.563935
H	-0.572226	-1.645279	3.932596
H	-0.516434	1.658816	3.935280
H	-0.048082	2.556915	2.489129
H	-1.655697	1.868611	2.619114
H	-0.981616	0.312068	-0.381544
H	0.724701	0.704760	-0.433321
H	0.199377	-0.981751	-0.446626
N	2.005500	-0.000824	2.376909
C	2.362740	-0.087786	3.798488
C	3.841534	-0.100645	4.095349
C	4.819685	-0.107589	3.198211
H	2.389961	-0.806331	1.857066
H	2.419661	0.837455	1.972557
H	1.890410	0.750669	4.322491
H	1.900064	-0.996081	4.200352
H	4.089209	-0.106740	5.155260
H	4.625169	-0.111152	2.130199
H	5.859714	-0.119132	3.504317
N	2.578594	-2.379944	0.625529
C	3.049658	-1.984020	-0.710587
C	2.709691	-2.971105	-1.800402
C	1.904791	-2.700788	-2.821569
H	1.584545	-2.595883	0.584158
H	3.048367	-3.225117	0.936664
H	2.609253	-1.011999	-0.951489
H	4.134931	-1.848318	-0.649771
H	3.146602	-3.964988	-1.703108
H	1.671380	-3.444608	-3.576033
H	1.450346	-1.719881	-2.934397

9IVAIV

Al	0.000008	0.000837	2.014592
C	1.751351	0.000078	2.986096
C	-1.749782	0.047298	2.987754
C	-0.000418	-0.001907	0.015381
H	2.384817	0.859317	2.726111
H	2.362049	-0.886983	2.768506
H	1.640276	0.027936	4.079395
H	-1.636740	0.071249	4.080947
H	-2.359907	0.923682	2.729199
H	-2.384659	-0.822629	2.770196
H	0.887220	0.501558	-0.393330
H	-0.017807	-0.995995	-0.450171
H	-0.869611	0.532442	-0.393692
N	-0.030249	-2.234038	2.065129
C	-0.037712	-2.841093	3.394942
C	-0.058535	-4.349860	3.445479
C	-0.070636	-5.172278	2.403527
H	-0.850615	-2.524185	1.538118
H	0.781179	-2.546519	1.537051
H	-0.906451	-2.448220	3.934539
H	0.842288	-2.472390	3.933348
H	-0.063622	-4.766516	4.451439
H	-0.085425	-6.247988	2.538610
H	-0.066355	-4.812673	1.379002
N	0.030238	2.237650	1.954688
C	0.040346	2.907307	3.254083
C	0.060573	4.416799	3.232792
C	0.070077	5.188662	2.152818
H	-0.782267	2.524613	1.414075
H	0.849211	2.502718	1.412652
H	-0.838278	2.564581	3.811574
H	0.910427	2.541153	3.810072
H	0.067571	4.880753	4.217833
H	0.063821	4.780572	1.146641
H	0.084661	6.269593	2.236565

9IVBIV

Al	0.003447	-0.000220	2.010179
C	1.720794	0.001558	3.034307
C	0.000623	0.005063	0.010893
C	-1.743497	-0.063323	2.982613
H	2.426543	0.764615	2.677501
H	1.553743	0.214519	4.099605
H	2.270353	-0.947844	3.003162
H	-0.280825	0.967974	-0.436264
H	-0.704334	-0.728421	-0.404454
H	0.985427	-0.242835	-0.408672
H	-1.652786	-0.533053	3.972569
H	-2.490726	-0.654224	2.433835
H	-2.214666	0.912399	3.159554
N	-0.011029	2.227643	2.011218
C	0.109061	2.892848	3.307275

C	-0.002804	4.398542	3.301867
C	-0.191527	5.169985	2.237794
H	-0.889159	2.480082	1.563555
H	0.731861	2.528891	1.384825
H	-0.659530	2.474532	3.967538
H	1.069781	2.600161	3.743492
H	0.084259	4.860786	4.283811
H	-0.260530	6.247708	2.333494
H	-0.284188	4.762908	1.235426
N	-0.026780	-2.257522	2.037125
C	0.941589	-2.959944	1.198247
C	0.942722	-4.467322	1.290240
C	0.149778	-5.208169	2.055164
H	-0.974664	-2.537086	1.796648
H	0.108325	-2.502775	3.015283
H	0.762801	-2.659630	0.160469
H	1.939194	-2.582453	1.449860
H	1.675582	-4.958082	0.651756
H	0.220564	-6.290082	2.053611
H	-0.598376	-4.770184	2.708963

9IVHIV

Al	0.024001	0.010098	1.991236
C	1.794710	-0.018944	2.864544
C	-1.369542	1.116999	2.857718
C	0.031380	0.031220	0.011208
H	2.338757	0.915507	2.675245
H	1.740818	-0.120439	3.956116
H	2.443548	-0.825648	2.498265
H	-1.330952	1.079350	3.953999
H	-2.394707	0.844643	2.570307
H	-1.251146	2.174475	2.587740
H	0.577085	0.908545	-0.360409
H	0.533558	-0.841178	-0.428900
H	-0.967030	0.087578	-0.442381
N	-0.674967	-1.880625	2.360619
C	-0.858314	-2.204958	3.781008
C	-1.390637	-3.585871	4.071486
C	-1.769256	-4.486492	3.172982
H	-1.569680	-1.949788	1.850024
H	-0.038845	-2.553377	1.936241
H	-1.533419	-1.454246	4.206851
H	0.103776	-2.069077	4.287192
H	-1.455396	-3.828878	5.130558
H	-2.140514	-5.457791	3.479947
H	-1.732755	-4.291580	2.105736
N	-3.157372	-1.531456	0.676092
C	-3.110966	-2.091739	-0.670032
C	-4.096013	-1.540762	-1.677871
C	-4.986936	-0.583349	-1.452209
H	-2.978525	-0.530170	0.646455
H	-4.080408	-1.654298	1.082293
H	-2.095292	-1.949638	-1.059242
H	-3.257153	-3.176127	-0.594897
H	-4.035594	-1.991927	-2.667238
H	-5.079653	-0.098776	-0.485208
H	-5.655666	-0.243839	-2.235234

10IAI

C	-0.001847	-0.000059	0.020490
Al	0.001653	-0.000241	2.015306
N	2.242748	-0.000162	1.962670
C	2.893656	0.000429	3.281499
C	4.362459	0.000495	3.222586
C	5.556840	0.000526	3.144376
C	0.024712	-1.745406	2.996974
N	-2.237380	-0.000302	2.074351
C	-2.824684	0.000231	3.422776
C	-4.294572	0.000229	3.433451
C	-5.491296	0.000224	3.411079
C	0.024620	1.744664	2.997417
H	2.544123	-0.878871	3.829220
H	2.539682	0.814061	1.430208
H	2.539751	-0.814754	1.430808
H	2.544019	0.880169	3.828463
H	-0.852715	2.369633	2.780778
H	0.050200	1.631469	4.090597
H	0.891384	2.368759	2.739686
H	-0.997004	0.000527	-0.442570
H	0.516871	0.878197	-0.388709
H	0.515887	-0.878858	-0.388802
H	-0.852564	-2.370382	2.780131
H	0.891494	-2.369403	2.739084
H	0.050259	-1.632515	4.090188
H	6.620778	0.000560	3.085649
H	-2.559444	0.814083	1.556798
H	-2.559401	-0.815072	1.557374
H	-2.449194	-0.879103	3.952967
H	-2.449205	0.880012	3.952249
H	-6.556820	0.000215	3.402276

10IBI

Al	-0.030090	-0.044403	1.963237
C	1.716666	-0.058176	2.937440
C	-0.022500	-0.027122	-0.033538
C	-1.748098	0.029225	2.983896
H	2.154132	-1.050255	3.110975
H	2.483651	0.503453	2.385514
H	1.647687	0.414435	3.927467
H	0.675231	0.716645	-0.441995
H	0.276147	-0.983950	-0.482506
H	-1.007716	0.207008	-0.460054
H	-2.483626	-0.709736	2.636547
H	-1.592039	-0.174225	4.052869
H	-2.263943	0.997058	2.942948

N	0.093941	2.215446	2.010178
C	-0.858146	2.945214	1.160783
C	-0.815745	4.404338	1.337585
C	-0.759630	5.587854	1.507419
H	1.046007	2.484642	1.775618
H	-0.045058	2.474922	2.984085
H	-0.648943	2.688615	0.119386
H	-1.863118	2.576181	1.384521
H	-0.715124	6.641901	1.656865
N	-0.117892	-2.250112	1.955460
C	-0.288459	-2.897803	3.265508
C	-0.204527	-4.364271	3.214826
C	-0.124795	-5.556164	3.139742
H	-0.860826	-2.543291	1.325078
H	0.754283	-2.558322	1.531505
H	-1.255670	-2.589503	3.669910
H	0.480567	-2.504151	3.936518
H	-0.052290	-6.617658	3.079917

10IHI

Al	0.000115	0.000013	1.978936
C	-0.569886	1.669870	2.864645
C	-0.542115	-1.700089	2.833405
C	0.000233	0.000392	-0.000120
H	-0.023848	2.552139	2.504799
H	-0.461115	1.648567	3.956753
H	-1.631254	1.871976	2.671044
H	-0.531321	-1.665932	3.930333
H	-1.567734	-1.968381	2.548603
H	0.085175	-2.552407	2.536219
H	0.697248	0.725909	-0.441309
H	0.239800	-0.981846	-0.428502
H	-0.991817	0.263652	-0.389398
N	2.016746	0.000038	2.352416
C	2.382136	-0.160019	3.773588
C	3.832739	-0.164496	4.000300
C	5.017678	-0.156090	4.165711
H	2.415001	-0.775582	1.799132
H	2.426963	0.860708	1.995198
H	1.943682	-1.096938	4.127667
H	1.919094	0.650974	4.343313
H	6.072183	-0.149436	4.319752
N	2.762210	-2.352820	0.602120
C	3.199959	-1.944986	-0.738273
C	3.314134	-3.049835	-1.705299
C	3.400562	-3.969913	-2.466273
H	1.840282	-2.778406	0.545281
H	3.387881	-3.064544	0.968292
H	2.490082	-1.203395	-1.117425
H	4.170410	-1.447532	-0.650039
H	3.471873	-4.783370	-3.150858

10IAII

C	0.000882	-0.006038	0.001072
Al	-0.001122	-0.000197	1.999767
N	2.259797	0.005296	1.973707
C	3.022383	0.239425	3.216051
C	3.151193	-0.985445	4.008771
C	3.287196	-1.989334	4.643547
C	-0.078164	-1.732939	2.979939
N	-2.233693	0.101575	1.948194
C	-2.872430	0.133287	3.272483
C	-4.338145	0.236101	3.226598
C	-5.530303	0.320975	3.160976
C	0.044704	1.769527	2.945126
H	-2.458027	0.981464	3.824110
H	-2.570982	-0.699275	1.419651
H	-2.493957	0.929128	1.416970
H	-2.579009	-0.773987	3.807386
H	0.747998	-2.400942	2.707618
H	-0.011118	-1.611595	4.069452
H	-1.001418	-2.295505	2.782851
H	0.969095	-0.232244	-0.465218
H	-0.697945	-0.750352	-0.405143
H	-0.312155	0.963224	-0.412387
H	0.901647	2.391945	2.652420
H	-0.841839	2.384468	2.738089
H	0.097466	1.676412	4.039173
H	-6.591684	0.399980	3.110418
H	2.580501	-0.848001	1.522720
H	2.432747	0.766235	1.321551
H	2.491151	0.998572	3.797308
H	4.029496	0.620852	3.008187
H	3.386943	-2.884343	5.212748

10IBII

Al	0.009607	0.006842	2.014862
C	-0.006930	-0.003190	0.011812
C	1.733227	0.004887	3.027155
C	-1.726996	-0.033893	2.985523
H	-0.512654	-0.884292	-0.407204
H	-0.530090	0.859699	-0.421414
H	1.002540	0.001621	-0.424321
H	2.530462	-0.552066	2.514422
H	1.600886	-0.475618	4.006627
H	2.154176	0.994907	3.243111
H	-1.578984	-0.075999	4.072651
H	-2.337276	-0.911048	2.736096
H	-2.362346	0.840558	2.789028
N	-0.051981	2.255305	2.030851
C	1.002319	2.944576	1.273656
C	0.918293	4.411294	1.332922
C	0.821533	5.602637	1.397546
H	-0.024459	2.543486	3.006360
H	-0.966321	2.526542	1.677770

H	1.968935	2.611784	1.661441
H	0.942885	2.611530	0.234213
H	0.744689	6.664221	1.448444
N	0.134940	-2.264371	1.891790
C	0.591501	-3.100242	3.016824
C	-0.368483	-3.082527	4.123374
C	-1.161088	-3.097667	5.018176
H	-0.782348	-2.572530	1.577743
H	0.768987	-2.384140	1.105555
H	1.549050	-2.700760	3.361495
H	0.752747	-4.142474	2.714098
H	-1.867282	-3.088638	5.815727

10IHII

Al	-0.003946	0.008975	1.990718
C	-0.042441	0.030422	0.010916
C	-1.401051	1.082602	2.887388
C	1.781468	-0.022097	2.834781
H	0.533670	-0.791004	-0.436270
H	0.392858	0.956984	-0.384730
H	-1.064111	-0.022218	-0.388598
H	-2.418931	0.794813	2.590924
H	-1.299543	2.143587	2.624158
H	-1.359183	1.037964	3.983136
H	2.303588	0.933119	2.694183
H	2.438633	-0.792731	2.410675
H	1.749872	-0.189600	3.919486
N	-0.654628	-1.898235	2.353526
C	-1.002574	-2.175332	3.760573
C	-1.443745	-3.557792	3.987995
C	-1.795353	-4.688647	4.159750
H	-1.465770	-2.092874	1.747065
H	0.058315	-2.559667	2.046082
H	-1.791046	-1.477712	4.055061
H	-0.129800	-1.958079	4.383348
H	-2.109469	-5.694357	4.319213
N	-2.701494	-2.639042	0.227010
C	-1.764671	-3.093980	-0.809597
C	-0.808878	-4.061380	-0.254303
C	-0.041990	-4.856166	0.206573
H	-3.300907	-3.402458	0.525309
H	-3.297097	-1.904275	-0.141441
H	-1.211395	-2.221014	-1.169432
H	-2.259930	-3.553160	-1.675582
H	0.640856	-5.569632	0.607058

10IIHI

Al	0.024550	-0.028701	1.981768
C	0.040551	-0.001276	-0.002026
C	-0.630442	1.620358	2.835775
C	-0.477485	-1.756789	2.802620
H	-0.959008	0.240870	-0.386159
H	0.711006	0.764262	-0.417181
H	0.313221	-0.958658	-0.465089
H	-0.202692	2.529731	2.393868
H	-1.719118	1.710517	2.726229
H	-0.418080	1.652501	3.910647
H	-0.452754	-1.740484	3.899777
H	-1.505055	-2.026218	2.526009
H	0.151690	-2.597716	2.478522
N	2.059672	-0.013373	2.328992
C	2.553289	-0.523948	3.628964
C	2.311432	0.426275	4.716382
C	2.134639	1.211598	5.600080
H	2.452693	-0.610745	1.584400
H	2.416837	0.929011	2.182112
H	3.626806	-0.738338	3.577324
H	2.031496	-1.461972	3.837472
H	1.956770	1.909767	6.385313
N	2.946146	-1.973360	0.174003
C	3.306573	-1.351979	-1.107320
C	3.425973	-2.297508	-2.229707
C	3.516671	-3.092082	-3.120469
H	2.033642	-2.414361	0.087491
H	3.604568	-2.716119	0.391294
H	2.546644	-0.601705	-1.345406
H	4.256840	-0.824144	-0.982808
H	3.593090	-3.791904	-3.920427

10IIAII

C	-0.011099	-0.002287	0.017991
Al	0.000296	0.000266	2.023602
C	1.772951	0.004318	2.939194
N	0.072668	-2.263412	2.014681
C	0.274653	-2.979629	3.291087
C	-0.995630	-3.261979	3.963886
C	-2.027772	-3.528841	4.505362
C	-1.741835	0.062129	2.985342
N	-0.035810	2.270612	1.879581
C	-0.415290	3.111407	3.030711
C	0.648330	3.154156	4.037621
C	1.522548	3.212646	4.851051
H	-0.644971	4.140176	2.726732
H	-0.710945	2.400892	1.129857
H	0.867137	2.566698	1.516591
H	-1.317627	2.682485	3.474148
H	-2.286541	-0.887600	2.957012
H	-1.635483	0.316792	4.048626
H	-2.417348	0.813064	2.550584
H	0.142253	-0.983646	-0.450292
H	-0.965362	0.367705	-0.384143
H	0.771727	0.646846	-0.399308
H	2.404844	-0.854184	2.670450
H	2.362056	0.896558	2.694126
H	1.688316	0.000726	4.033986

H	2.301749	3.246409	5.576782
H	-0.728452	-2.646106	1.518938
H	0.884433	-2.403415	1.419106
H	0.899702	-2.350769	3.932081
H	0.798488	-3.931438	3.142222
H	-2.948260	-3.743680	4.996986

10IIBII

Al	-0.044211	0.092531	1.980148
C	0.003329	1.813274	2.997197
C	-0.013816	-1.637514	2.972676
C	-0.105973	0.085174	-0.014328
H	0.669770	2.535204	2.508202
H	-0.962229	2.323625	3.114082
H	0.393287	1.676768	4.016624
H	0.964900	-2.130885	3.047318
H	-0.369369	-1.530470	4.006431
H	-0.682811	-2.371903	2.504505
H	0.431621	-0.775766	-0.435999
H	0.357816	0.984100	-0.442163
H	-1.116635	0.035768	-0.440459
N	-2.292430	0.125764	2.048399
C	-2.932381	0.117898	3.381619
C	-3.376161	-1.226513	3.756194
C	-3.757694	-2.323291	4.041547
H	-2.484373	1.004838	1.576558
H	-2.677644	-0.614133	1.468196
H	-2.203937	0.482744	4.113275
H	-3.798189	0.788932	3.414434
H	-4.083317	-3.302960	4.304889
N	2.247801	0.111200	1.939308
C	3.014221	0.592041	0.774901
C	2.891163	2.042704	0.607733
C	2.821810	3.229200	0.477390
H	2.526424	0.623766	2.772978
H	2.466947	-0.866950	2.105578
H	4.079940	0.343814	0.855938
H	2.618537	0.094546	-0.114718
H	2.738825	4.284776	0.359327

10IIHII

Al	0.000237	-0.000084	1.985905
C	0.001392	0.002468	-0.000008
C	-0.673785	1.643601	2.834540
C	-0.488526	-1.725438	2.824772
H	-1.010895	0.183921	-0.384081
H	0.629645	0.794611	-0.430367
H	0.323645	-0.950420	-0.440785
H	-0.143615	2.544784	2.500533
H	-1.732725	1.799505	2.589386
H	-0.604294	1.619265	3.928176
H	-1.499769	-2.028769	2.523965
H	0.174590	-2.551030	2.530547
H	-0.496393	-1.694730	3.921809
N	2.025635	0.001901	2.317500
C	2.506773	-0.261228	3.693536
C	2.409289	0.928434	4.541873
C	2.352753	1.906612	5.226832
H	2.383273	-0.744689	1.701573
H	2.447068	0.865705	1.978009
H	1.896868	-1.066926	4.112557
H	3.548514	-0.600107	3.676645
H	2.279051	2.775972	5.838638
N	3.002035	-1.999911	0.251012
C	3.433018	-1.034785	-0.769265
C	4.441635	-0.118529	-0.219412
C	5.266407	0.619775	0.235639
H	2.204609	-2.530261	-0.086589
H	3.746658	-2.657772	0.458775
H	2.554865	-0.455234	-1.071421
H	3.842046	-1.504772	-1.673258
H	6.003881	1.282339	0.626798

methylamine

N	0.106446	0.744389	0.000000
C	-0.018492	-0.711052	0.000000
H	-0.342100	1.147219	-0.815007
H	-0.342100	1.147219	0.815007
H	0.488676	-1.114171	0.879892
H	0.488676	-1.114171	-0.879892
H	-1.051892	-1.085624	0.000000

n-propylamine I

N	1.948920	0.034236	0.000000
C	0.592437	-0.503306	0.000000
C	-0.542072	0.534015	0.000000
C	-1.929388	-0.121137	0.000000
H	2.105951	0.617489	-0.815477
H	2.105951	0.617489	0.815477
H	0.486875	-1.152668	-0.876448
H	0.486875	-1.152668	0.876448
H	-0.434201	1.180500	-0.879430
H	-0.434201	1.180500	0.879430
H	-2.062783	-0.753092	-0.883610
H	-2.062783	-0.753092	0.883610
H	-2.725735	0.627491	0.000000

n-propylamine II

N	0.028823	-0.024676	0.022938
C	-0.004845	-0.040947	1.483729
C	1.414244	-0.006526	2.055568
C	1.423332	0.009215	3.588600
H	0.481148	-0.860069	-0.334653

H	-0.907089	-0.002363	-0.366906
H	-0.545889	0.851675	1.816849
H	-0.536849	-0.911374	1.901073
H	1.927904	0.875195	1.659531
H	1.966355	-0.882230	1.691649
H	0.921502	-0.874245	3.995795
H	0.905832	0.893767	3.973015
H	2.443911	0.024110	3.979850

n-propylamine III

C	0.015407	0.000669	1.465091
C	1.397049	0.006911	2.145999
C	2.223502	-1.252051	1.854674
H	0.459599	-0.838499	-0.361390
H	0.509145	0.794921	-0.364601
H	-0.548643	-0.876234	1.803437
H	-0.550895	0.878346	1.793178
H	1.951086	0.897322	1.823456
H	1.249836	0.104197	3.228180
H	1.685239	-2.151034	2.173159
H	3.180757	-1.230798	2.382210
H	2.441545	-1.351078	0.787100

n-propylamine IV

N	0.138805	-0.031095	0.038945
C	0.032475	-0.070149	1.497380
C	1.420465	-0.022908	2.148647
C	2.175522	1.281210	1.864537
H	-0.774536	0.049438	-0.393612
H	0.560539	-0.885342	-0.311882
H	-0.540823	0.808787	1.812797
H	-0.507206	-0.955356	1.867251
H	1.300861	-0.159403	3.229147
H	2.008117	-0.878421	1.791560
H	1.624661	2.139978	2.261660
H	2.296435	1.429329	0.789607
H	3.165691	1.273486	2.328455

n-propylamine V

N	0.046409	-0.051107	0.023643
C	-0.005483	-0.039427	1.485319
C	1.402315	0.004852	2.088683
C	2.239486	-1.236864	1.752834
H	-0.881251	0.050036	-0.372637
H	0.418690	-0.929437	-0.320444
H	-0.551743	0.859028	1.788400
H	-0.546355	-0.903071	1.906226
H	1.911640	0.902970	1.724405
H	1.309551	0.098373	3.176377
H	2.438774	-1.304256	0.679434
H	3.207052	-1.209274	2.260962
H	1.723881	-2.151983	2.064136

cyclopropylamine I

N	0.223623	1.466774	0.000000
C	-0.492515	0.219962	0.000000
C	0.137706	-0.931946	-0.763497
C	0.137706	-0.931946	0.763497
H	0.004977	2.021525	0.820546
H	0.004977	2.021525	-0.820546
H	-1.582224	0.252390	0.000000
H	1.080570	-0.724017	-1.255407
H	-0.515968	-1.626582	-1.277803
H	1.080570	-0.724017	1.255407
H	-0.515968	-1.626582	1.277803

cyclopropylamine II

N	0.003992	-0.012563	0.007873
C	0.011849	-0.016241	1.445815
C	1.297684	-0.016389	2.273476
C	0.419046	1.236277	2.184909
H	0.639923	0.683846	-0.364362
H	0.281521	-0.914478	-0.365305
H	-0.824041	-0.566577	1.866701
H	2.235404	-0.001392	1.727968
H	1.320177	-0.561812	3.210478
H	0.789170	2.065161	1.589974
H	-0.149287	1.533213	3.058321

allylamine I

N	0.007201	-0.001265	0.004693
C	0.016188	-0.008913	1.468373
C	1.393192	-0.010207	2.090776
C	1.862546	-0.971950	2.878043
H	0.407077	0.858057	-0.357550
H	0.568571	-0.766088	-0.355975
H	-0.543724	0.870639	1.804684
H	-0.537758	-0.887679	1.812939
H	2.031294	0.837868	1.840547
H	2.866042	-0.936768	3.288918
H	1.251600	-1.831723	3.141438

allylamine II

N	0.043267	-0.027303	0.019196
C	-0.009010	-0.059878	1.480926
C	1.388130	-0.018645	2.041714
C	1.883248	-0.913563	2.888689
H	0.477185	-0.870510	-0.341350
H	-0.886132	0.036425	-0.380905
H	-0.549708	0.836488	1.807249
H	-0.540138	-0.930275	1.893781

H	2.005281	0.806436	1.691202
H	2.897803	-0.838408	3.265552
H	1.286957	-1.751994	3.239080

allylamine III

C	1.843961	-0.941392	2.885872
C	1.373308	-0.034127	2.040192
C	-0.025979	-0.021220	1.482833
N	0.006255	0.018092	0.017448
H	0.488844	0.850284	-0.307035
H	-0.934647	0.056927	-0.360005
H	-0.571493	0.830412	1.922169
H	-0.544965	-0.933352	1.791260
H	2.021383	0.780127	1.715470
H	2.857903	-0.890203	3.267768
H	1.228182	-1.769546	3.225670

allylamine IV

N	1.454356	-0.569251	0.000000
C	0.698537	0.670581	0.000000
C	-0.814622	0.578029	0.000000
C	-1.526200	-0.542771	0.000000
H	1.238925	-1.129349	0.817617
H	1.238925	-1.129349	-0.817617
H	1.008379	1.259552	-0.871936
H	1.008379	1.259552	0.871936
H	-1.332611	1.536552	0.000000
H	-2.610428	-0.521801	0.000000
H	-1.053337	-1.519996	0.000000

allylamine V

N	0.078612	-0.091940	0.016570
C	0.013399	-0.047220	1.470088
C	1.375855	-0.015182	2.116575
C	2.536322	0.068770	1.477000
H	0.496673	-0.961903	-0.297486
H	-0.848530	-0.035539	-0.388123
H	-0.527689	0.862849	1.758676
H	-0.548129	-0.886866	1.912937
H	1.366436	-0.075336	3.203622
H	2.582806	0.146978	0.396188
H	3.473881	0.081436	2.022175

propargylamine I

N	1.593826	-0.449710	0.000000
C	0.597665	0.618937	0.000000
C	-0.808535	0.168615	0.000000
C	-1.937081	-0.233221	0.000000
H	1.470432	-1.042484	0.814290
H	1.470432	-1.042484	-0.814290
H	0.767148	1.250711	0.876959
H	0.767148	1.250711	-0.876959
H	-2.941883	-0.587078	0.000000

propargylamine II

N	0.032894	0.031565	0.018407
C	-0.002210	0.036264	1.481811
C	1.356568	0.004780	2.036658
C	2.463878	0.005217	2.489953
H	0.572493	0.818278	-0.326130
H	-0.906430	0.112296	-0.355880
H	-0.535756	-0.860280	1.814399
H	-0.524291	0.902367	1.915657
H	3.450718	-0.006284	2.890536

References

(S1) Marstokk, K.-M.; Møllendal, H. *Acta Chem. Scand. A* **1984**, *38*, 387.

(S2) Hendricksen, D. K.; Harmony, M. D. *J. Chem. Phys.* **1969**, *51*, 700.

(S3) (a) Roussy, G.; Demaison, J.; Botskor, I.; Rudolph, H. D. *J. Mol. Spectrosc.* **1971**, *38*, 535; (b) Botskor, I.; Rudolph, H. D.; Roussy, G. *J. Mol. Spectrosc.* **1974**, *53*, 15; (c) Botskor, I.; Rudolph, H. D.; Roussy, G. *J. Mol. Spectrosc.* **1974**, *52*, 457; (d) Botskor, I.; Rudolph, H. D. *J. Mol. Spectrosc.* **1978**, *71*, 430.

(S4) Cervellati, R.; Caminati, W.; Degli Esposti, C.; Mirri, A. M. *J. Mol. Spectrosc.* **1977**, *66*, 389.

(S5) (a) Simon, S.; Duran, M.; Dannenberg, J. J. *J. Chem. Phys.* **1996**, *105*, 11024; (b) Boys, S. F.;

Bernardi, F. *Mol. Phys.* **1970**, *19*, 553; (c) Boys, S. F.; Bernardi, F. *Mol. Phys.* **1976**, *19*, 325.