

AM1 CI, STO-3G, and 6-31G Study of Amino Derivatives of Diazaphenanthrenes

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For aminodiazaphenanthrenes and acylaminodiazaphenanthrenes UV spectral values, total energy, and effective charges have been calculated by the AM1 CI 12 method, and the geometry optimized. Correlations of experimental and calculated wavenumber values of considered compounds show good compatibility. In the case of aminodiazaphenanthrenes total energy and effective charges, along with geometry optimization have been also calculated by the STO-3G and 6-31G double ξ MP2 methods and the results have been compared.

In a continuation of the study concerning correlations of experimental and calculated UV spectral values of diazaphenanthrenes (daps) *I–III* along with those of their *N*-derivatives – quaternary salts with dihaloalkanes [1] and *N*-oxides [2] as well as *C*-derivatives – formyl- [3] and methyl daps [4], in the present paper such correlations for aminodaps *IV–VI* and their acyl derivatives, *i.e.* acetamido- *VII*, *IX* and benzamido-daps *VIII*, *X* are described.

Daps are interesting for their reactivity [5–8] and biological activities [9, 10]; aminodaps, a topic of this work are synthons of azo dyes [11] and of condensed four-ring azaaromatics [12, 13].

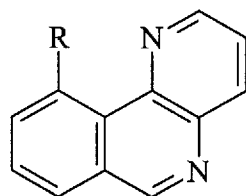
The AM1 CI 12 method (next referred to as AM1) has been used for correlations of experimental and theoretical UV spectroscopic results and for calculation of total energy, dipole moments, and effective charges as well as for geometry optimization [14]. In the case of *IV–VI* total energy and dipole moments calculations and geometry optimization were also made by the *ab initio* STO-3G [15] and 6-31G double ξ MP2 (next referred to as 6-31G) [16] methods. In a former work experimental UV data of *IV–VI* and their correlations with values calculated by the PPP method have been reported [17]. The results obtained by all methods used have been compared.

The experimental and calculated by the AM1 method UV spectral data of *IV–X* are given in Table 1. The experimental wavenumbers of the α -band of daps *I–III* [17], aminodaps *IV–VI* [17], and acylaminodaps *VII–X* increase in the order: aminodaps, daps, acylaminodaps. Comparison of $\log \{\epsilon\}$ values of α -, *p*-, and

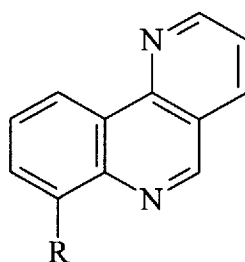
Table 1. Experimental UV Data Calculated by AM1 Wavenumber and Oscillator Strength Values in the Dipole Length Approximation for *IV–X*

Compound Band	Experimental		Calculated	
	$\bar{\nu} \cdot 10^3 / \text{cm}^{-1}$	$\log\{\epsilon\}$	$\bar{\nu} \cdot 10^3 / \text{cm}^{-1}$	f
<i>IV</i>				
α	25.1	3.784	24.455	0.153
<i>p</i>	38.1	4.070	38.897	0.787
β	41.7	4.547	42.642	0.318
<i>V</i>				
α	25.6	3.519	25.398	0.156
<i>p</i>	35.0	3.980	36.567	0.579
β	40.9	4.628	39.077	0.540
<i>VI</i>				
α	25.3	3.473	25.673	0.124
<i>p</i>	35.0	3.892	36.336	0.632
β	41.0	4.665	39.237	0.410
<i>VII</i>				
α	31.0	3.892	31.055	0.337
<i>p</i>	42.0	4.772	42.171	0.513
β	46.0	3.903	46.214	0.959
<i>VIII</i>				
α	31.0	4.215	30.968	0.307
<i>p</i>	42.0	4.760	43.397	0.391
β	45.5	3.857	45.984	0.584
<i>IX</i>				
α	36.0	4.477	35.409	0.225
<i>p</i>	39.5	4.663	39.469	0.192
β	41.5	4.940	41.457	1.021
<i>X</i>				
α	34.5	3.017	34.337	0.225
<i>p</i>	41.0	3.274	41.157	1.023
β	46.0	2.881	46.121	0.419

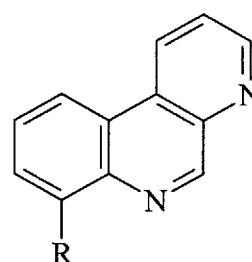
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<i>I</i>	R
<i>IV</i>	H
<i>VII</i>	NH ₂
<i>VIII</i>	NHCOMe
	NHCOPh



<i>II</i>	R
<i>V</i>	H
	NH ₂



<i>III</i>	R
<i>VI</i>	H
<i>IX</i>	NH ₂
<i>X</i>	NHCOMe
	NHCOPh

Table 2. Differences in the Experimental Wavenumber Values of α -, p -, and β -Bands for *IV*–*X* as Compared with Corresponding Parent Daps *I*–*III*, along with Experimental Wavenumber Values for *I*–*III*

Band	$\bar{\nu}(\text{difference}) \cdot 10^3/\text{cm}^{-1}$						
	<i>IV/I</i>	<i>V/II</i>	<i>VI/III</i>	<i>VII/I</i>	<i>VIII/I</i>	<i>IX/III</i>	<i>X/III</i>
α	+2.5	+3.5	+3.7	-3.4	-3.4	-7.0	-5.5
p	0.0	+3.2	+3.1	-3.9	-3.9	-1.4	-2.9
β	+0.5	+2.7	+2.3	-3.8	-3.3	+1.8	-2.7

Positive values denote red, negative blue shifts.

Experimental Wavenumber Values for *I*–*III* [17]

Band	$\bar{\nu} \cdot 10^3/\text{cm}^{-1}$		
	<i>I</i>	<i>II</i>	<i>III</i>
α	27.6	29.1	29.0
p	38.1	38.2	38.1
β	42.2	43.6	43.3

β -bands of *IV*–*VI* with those for parent daps shows the analogous increased order of $\log \{\epsilon\}$ value as that occurring in daps, *i.e.* α , p , β .

The differences between experimental wavenumber values of *IV*–*X* and those for corresponding unsubstituted daps [17] are shown in Table 2. Comparing wavenumber values of *IV*–*X* with those of parent daps, for α -, p -, and β -bands of *IV*–*VI* the red shift is observed (except for p -band of *IV*, where no shift takes place); in the case of *VII*–*X*, for all bands blue shifts occur (except for β -band of *IX*).

The correlations of observed and calculated by AM1 wavenumber values are:

For *IV*–*VI* $a = 1.2340$ $b = 1.2504$ $r = 0.9901$

For *VII* and *IX* $a = 1.0241$ $b = -0.9843$ $r = 0.9976$

For *VIII* and *X* $a = 1.0412$ $b = -1.3209$ $r = 0.9935$

Comparison of correlation coefficients for wavenumbers of *IV*–*VI* obtained with AM1 ($r = 0.9901$) and PPP [17] ($r = 0.9898$) methods shows a higher r value in the former case.

The correlations of observed and calculated wavenumber values for *IV*–*X* with corresponding unsubstituted daps *I*–*III* are:

Table 3. Total Energy, Binding Energy, Core Interaction Energy, Heat of Formation, and Dipole Moments Values for *IV*–*X* Calculated by the AM1 Method

Quantity	<i>IV</i>	<i>V</i>	<i>VI</i>	<i>VII</i>	<i>VIII</i>	<i>IX</i>	<i>X</i>
Total energy/eV	-2280.908	-2280.983	-2280.981	-2885.113	-3552.273	-2885.125	-3552.372
Binding energy/eV	-120.579	-120.654	-120.652	-144.058	-184.128	-144.071	-146.104
Core interaction energy/eV	10850.831	10735.726	10734.175	14937.708	21078.095	14660.723	20442.662
Heat of formation/eV	3.422	3.347	3.349	1.872	3.387	1.860	3.288
Dipole moments							
M_x/D	1.044	-1.143	1.904	-1.863	-2.738	2.678	0.336
M_y/D	-1.663	0.874	-0.756	2.146	1.038	-4.781	1.425
M_z/D	0.000	0.000	0.000	0.252	0.716	2.871	-0.750
$M(M)/D$	1.964	1.439	2.040	2.853	3.015	6.187	1.645

Table 4. Total Energy, Electronic Kinetic Energy, Nuclear Repulsion Energy, and Dipole Moments Values for IV—VI Calculated by the STO-3G and 6-31G Methods

Quantity	IV		V		VI	
	STO-3G	6-31G	STO-3G	6-31G	STO-3G	6-31G
Total energy/eV	-16763.017	-17017.361	-16748.809	-17017.345	-16748.755	-17017.244
Electronic kinetic energy/eV	16401.843	16940.593	16590.511	16940.925	16590.547	16940.562
Sum of electronic kinetic energy, electron—electron and electron— nucleus interaction energy/eV	-41693.764	-41771.385	-41113.574	-41553.379	-41082.583	-41523.629
Nuclear repulsion energy / eV	24930.746	24811.742	24364.765	24593.684	24333.827	24564.038
Dipole moments						
M_x/D	0.041	0.836	-1.481	-2.336	1.665	1.399
M_y/D	-1.613	-1.369	0.565	-0.273	-1.257	-1.615
M_z/D	0.001	0.001	0.008	1.062	0.001	0.004
$M(M)/D$	1.614	1.604	1.586	2.580	2.086	2.136

For IV/I $a = 1.0652$ $b = -1.1221$ $r = 0.9843$
 For V/II $a = 0.9805$ $b = 0.6395$ $r = 0.9697$
 For VI/III $a = 0.9486$ $b = 1.7395$ $r = 0.9797$
 For VII/I $a = 0.9633$ $b = 2.4664$ $r = 0.9783$
 For VIII/I $a = 0.9960$ $b = 1.4662$ $r = 0.9826$
 For IX/III $a = 1.0221$ $b = -0.7991$ $r = 0.9874$
 For X/III $a = 1.0165$ $b = -0.4687$ $r = 0.9937$

In correlations of experimental and calculated wave-number values of IV—VI and corresponding daps, the highest r has been found for IV/I ($r = 0.9843$); among correlations of acylaminodaps r is the highest for X/III ($r = 0.9937$).

For comparison, such correlation coefficients obtained with the use of the PPP method [17] are: for IV/I $r = 0.9826$; for V/II $r = 0.9917$; for VI/III $r = 0.9923$.

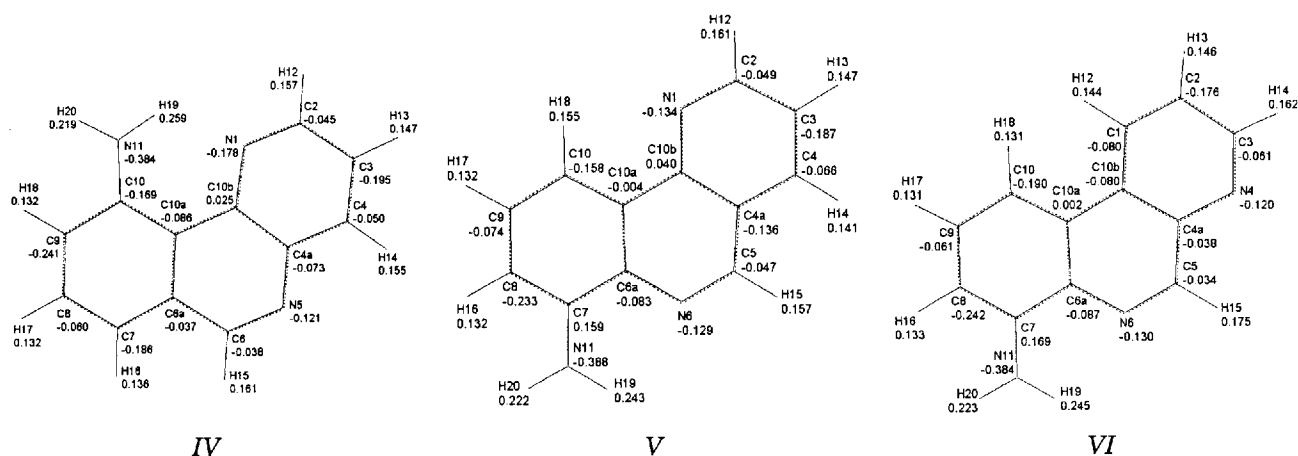
The total energy and dipole moment values for IV—X calculated by the AM1 method are given in Table 3 and those for IV—VI calculated by STO-3G and 6-31G methods in Table 4. In AM1 calculations, among three

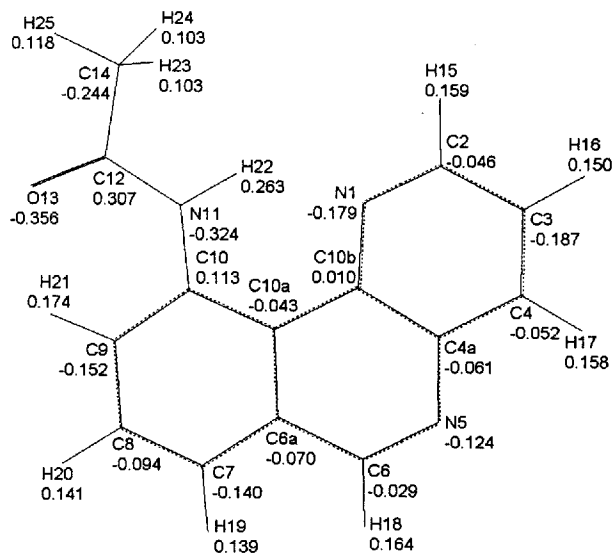
aminodaps IV—VI, the lowest total energy value, *i.e.* the highest stability, was found for V and the highest total energy value for IV. In the analysis of total energy values of IV—VI calculated by both STO-3G and 6-31G methods, the lowest value was found for IV, and the highest one for VI (Table 4).

In calculations by the AM1 method, the increased order of total dipole moment values of IV—VI is V, IV, VI, and among VII—X the sequence is X, VII, VIII, IX. Dipole moments of IV—VI calculated by the STO-3G method increase in the order V, IV, VI, as in the case of the AM1 method, whereas the 6-31G calculation shows the sequence IV, VI, V.

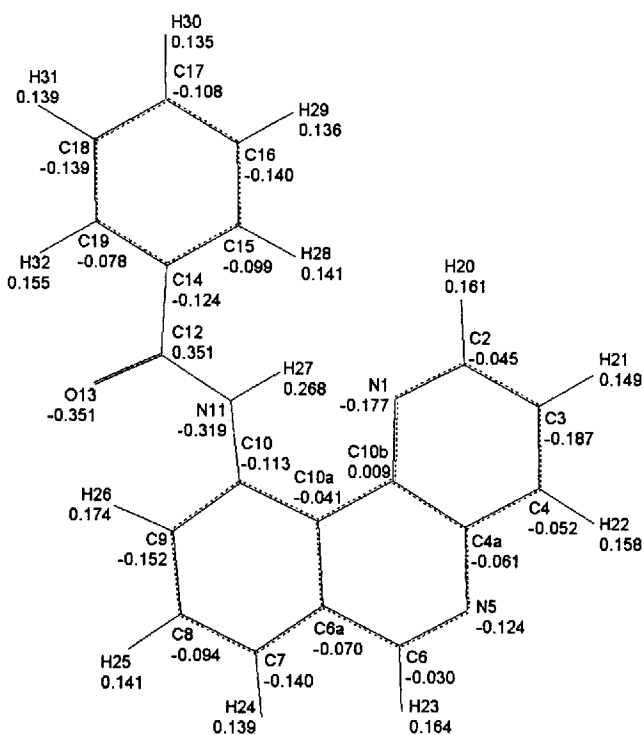
Effective charge values for IV—VI and VII—X calculated by the AM1 method are shown in Figs. 1 and 2, respectively, and those for IV—VI calculated by the STO-3G and 6-31G methods are given in Fig. 3.

In all the calculations for IV—VI, among three nitrogen atoms, the lowest effective charge values were found at amino group, and in the carbocyclic ring at

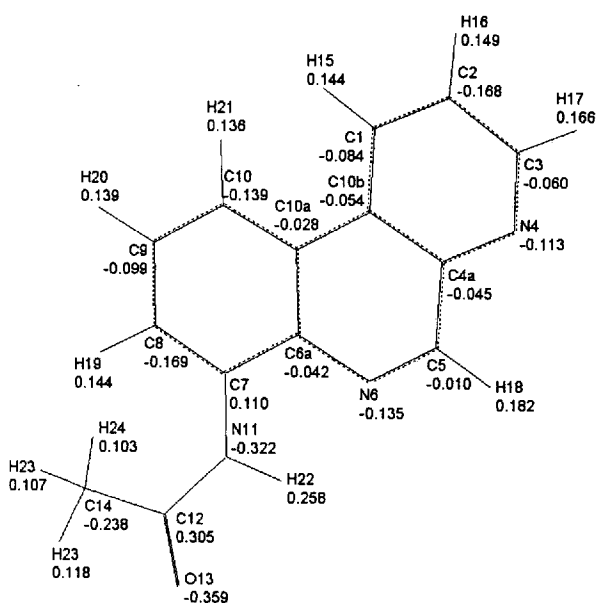
**Fig. 1.** Effective charge numerical values for IV—VI calculated by the AM1 method.



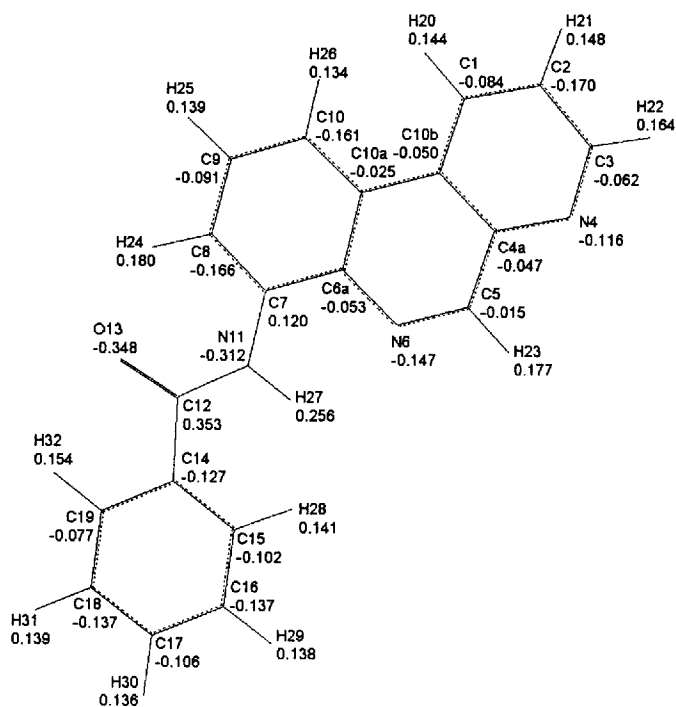
VII



VIII



IX



X

Fig. 2. Effective charge numerical values for VII—X calculated by the AM1 method.

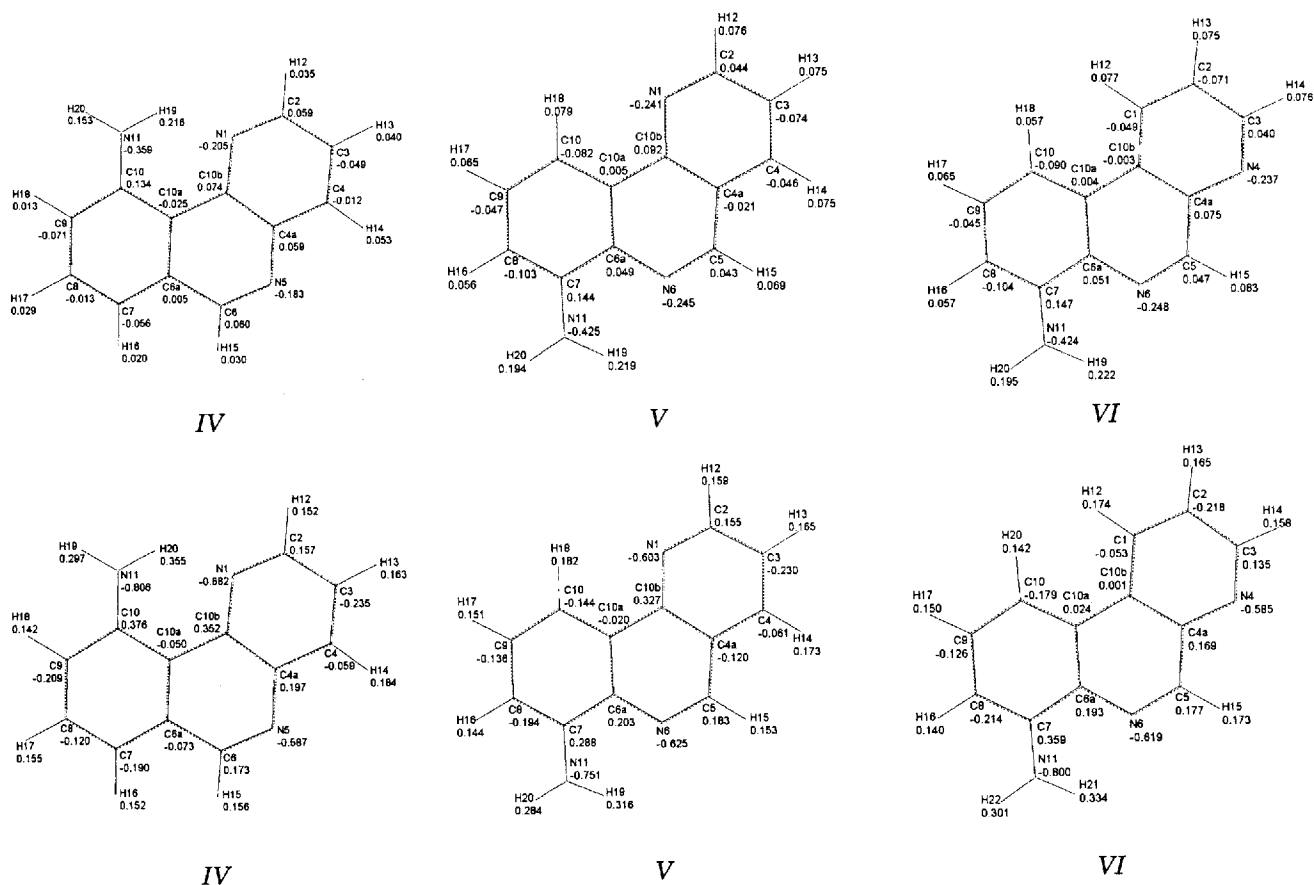


Fig. 3. Effective charge numerical values for IV–VI calculated by the STO-3G (top line) and 6-31G (bottom line) methods.

ortho and *para* positions relative to the amino group, these positions being influenced by the electron-donating character of the substituent.

AM1 calculations of effective charges of acylaminodaps VII–X have shown, as in the case of aminodaps, the lowest effective charge values for nitrogen atoms of acylamino group, and in carbocyclic rings at *ortho* and *para* positions to the acylamino groups.

Geometry optimization for IV–VI calculated by the AM1, STO-3G, and 6-31G methods is given in Table 5, and that for VII–X calculated by the AM1 method in Table 6.

Analyzing geometry optimization calculated by the AM1 method in IV and V, the 10a–10b bonds are the longest, and 5–6 bonds the shortest; in VI bonds 4a–5 and 6a–7 are longer than the other ones (Table 5). For IV and V the angles at the positions 6 and 2 and 5 and 2, respectively, are higher than the other ones; in the case of VI, however, higher angles are at the positions 5 and 3.

For 1,5-dap derivatives VII and VIII the longest are 10a–10b and the shortest 5–6 bonds. In 4,6-dap derivatives IX and X the longest bonds are 4a–6, and the shortest ones 5–6 bonds, similarly as for VII and VIII. For VII and VIII the angles at the position 6 are the

biggest, and angles 6a–10a–10b the smallest; similar sequence is found for the parent aminodap IV. In IX and X angles at the position 5 are the biggest and angles 10b–4a–5 the smallest; similar sequence was found for parent aminodap VI.

Analyzing geometry optimization calculated by the STO-3G and 6-31G methods, for IV the bonds C10a–C10b and C6–C6a are longer than the other ones, and N5–C6 bonds are the shortest. In V and VI the bonds C10a–C10b and C4a–C5 are longer than the other ones, and C5–C6 bonds are the shortest. Higher than the other ones for IV are angles at C6 and C2, for V angles at C2 and C5 and for VI the angle N4–C4a–C10b and angle at C5.

The above deformations of the hexagonal structure of three rings of IV–X shown by all the calculations used are due to the presence of nitrogen atoms and amino or acylamino substituents.

EXPERIMENTAL

The UV spectra of compounds have been recorded in 1,2-dichloroethane solution ($c = 10^{-4}$ mol dm⁻³) on a UV VIS Specord spectrophotometer. Calculations were made by the AM1 CI 12, STO-3G, and 6-31G methods.

Table 5. Bond Lengths and Angles for IV-VI Calculated by the AM1, STO-3G, and 6-31G Methods

Bond	IV			V			VI		
	AM1	STO-3G	6-31G	AM1	STO-3G	6-31G	AM1	STO-3G	6-31G
Length/Å									
N1-C2	1.329	1.301	1.306	1.331	1.329	1.302	1.381	1.362	1.364
C2-C3	1.416	1.392	1.395	1.421	1.415	1.405	1.420	1.414	1.406
C3-C4	1.379	1.345	1.369	1.381	1.362	1.364	1.331	1.328	1.299
C4-C4a	1.424	1.397	1.398	1.411	1.414	1.404	1.368	1.384	1.343
C4a-C10b	1.440	1.385	1.403	1.424	1.393	1.395	1.424	1.394	1.393
C10b-N1	1.368	1.359	1.342	1.372	1.384	1.342	1.416	1.417	1.409
C4a-N5	1.393	1.399	1.378	1.444	1.459	1.439	1.462	1.462	1.442
N5-C6	1.303	1.269	1.271	1.304	1.298	1.273	1.302	1.297	1.272
C6-C6a	1.452	1.446	1.448	1.395	1.422	1.379	1.394	1.422	1.377
C6a-C10a	1.416	1.383	1.403	1.425	1.397	1.398	1.424	1.399	1.398
C10a-C10b	1.460	1.454	1.456	1.460	1.467	1.450	1.445	1.469	1.454
C6a-C7	1.402	1.388	1.397	1.449	1.431	1.420	1.449	1.432	1.424
C7-C8	1.385	1.352	1.372	1.410	1.380	1.376	1.410	1.380	1.380
C8-C9	1.389	1.377	1.388	1.393	1.401	1.400	1.392	1.399	1.396
C9-C10	1.419	1.371	1.390	1.384	1.369	1.367	1.384	1.368	1.369
C10-C10a	1.440	1.418	1.427	1.404	1.409	1.404	1.406	1.412	1.407
C10-N11	1.369	1.364	1.359	1.373	1.394	1.384	1.371	1.393	1.361
Angle/°									
N1-C2-C3	124.011	124.320	123.717	124.371	124.719	124.229	118.734	119.344	118.919
C2-C3-C4	118.255	118.084	117.688	118.204	118.853	118.001	123.759	124.189	123.239
C3-C4-C4a	119.443	119.594	119.567	118.940	118.740	118.854	117.448	115.616	117.982
C4-C4a-C10b	118.554	118.685	118.559	119.249	118.722	118.453	123.215	124.334	124.027
C4a-C10b-N1	120.436	121.229	120.807	121.342	123.151	122.218	117.312	117.408	116.621
C10b-N1-C2	119.302	118.088	119.663	117.894	115.814	118.244	119.530	119.107	119.211
C4a-N5-C6	117.789	116.237	117.909	124.380	125.083	123.844	123.992	124.846	123.432
N5-C6-C6a	125.075	126.254	125.238	119.035	116.747	119.216	119.667	116.643	119.562
C6-C6a-C10a	118.898	118.288	118.485	122.388	123.727	123.103	120.015	124.087	123.272
C6a-C10a-C10b	117.092	116.960	116.548	117.995	117.788	117.209	118.055	117.637	116.821
C10a-C10b-C4a	118.297	118.625	118.445	117.994	118.198	118.187	119.167	117.944	118.375
C10b-C4a-N5	122.849	123.636	123.374	118.217	118.457	118.425	117.093	118.843	118.537
C6a-C7-C8	119.526	119.473	118.641	118.442	119.106	118.533	118.380	119.265	118.629
C7-C8-C9	120.364	120.652	120.736	121.069	120.250	120.907	120.958	119.921	120.361
C8-C9-C10	121.700	121.547	122.001	121.171	121.393	121.316	121.198	121.536	121.716
C9-C10-C10a	118.446	118.468	118.092	119.995	119.625	118.924	120.281	120.098	119.330
C10-C10a-C6a	117.890	118.731	118.495	120.498	119.893	120.412	120.021	119.072	119.576
C10a-C6a-C7	122.074	121.128	122.035	118.826	119.732	119.896	119.161	120.109	120.387
C9-C10-N11	118.023	120.749	119.617	121.422	118.399	119.419	121.427	118.230	118.946

Table 6. Bond Lengths and Angles for VII—X Calculated by the AM1 Method

VII		VIII		IX		X	
Length/Å		Length/Å		Length/Å		Length/Å	
N1—C2	1.328	N1—C2	1.328	C1—C2	1.381	C1—C2	1.381
C2—C3	1.417	C2—C3	1.417	C2—C3	1.421	C2—C3	1.421
C3—C4	1.379	C3—C4	1.378	C3—N4	1.331	C3—N4	1.330
C4—C4a	1.425	C4—C4a	1.425	C4—C4a	1.368	C4—C4a	1.368
C4a—C10b	1.440	C4a—C10b	1.439	C4a—C10b	1.424	C4a—C10b	1.424
C10b—N1	1.368	C10b—N1	1.368	C10b—C1	1.416	C10b—C1	1.416
C4a—N5	1.393	C4a—N5	1.393	C4a—C5	1.463	C4a—C5	1.462
N5—C6	1.303	N5—C6	1.303	C5—N6	1.302	C5—N6	1.301
C6—C6a	1.451	C6—C6a	1.451	N6—C6a	1.396	N6—C6a	1.396
C6a—C10a	1.416	C6a—C10a	1.416	C6a—C10a	1.424	C6a—C10a	1.424
C10a—C10b	1.464	C10a—C10b	1.464	C10a—C10b	1.445	C10a—C10b	1.415
C6a—C7	1.404	C6a—C7	1.404	C6a—C7	1.447	C6a—C7	1.451
C7—C8	1.381	C7—C8	1.381	C7—C8	1.399	C7—C8	1.400
C8—C9	1.395	C8—C9	1.395	C8—C9	1.399	C8—C9	1.398
C9—C10	1.408	C9—C10	1.408	C9—C10	1.380	C9—C10	1.380
C10—C10a	1.439	C10—C10a	1.439	C10—C10a	1.408	C10—C10a	1.407
C10—N11	1.400	C10—N11	1.401	C7—N11	1.401	C7—N11	1.401
N11—C12	1.392	N11—C12	1.392	N11—C12	1.393	N11—C12	1.391
C12—O13	1.245	C12—O13	1.246	C12—O13	1.246	C12—O13	1.245
C12—C14	1.512	C12—C14	1.494	C12—C14	1.503	C12—C14	1.494
		C14—C15	1.398			C14—C15	1.398
		C15—C16	1.395			C15—C16	1.395
		C16—C17	1.395			C16—C17	1.395
		C17—C18	1.395			C17—C18	1.395
		C18—C19	1.394			C18—C19	1.394
		C19—C14	1.400			C19—C14	1.400
Angle/°		Angle/°		Angle/°		Angle/°	
N1—C2—C3	123.927	N1—C2—C3	123.887	C1—C2—C3	118.775	C1—C2—C3	118.783
C2—C3—C4	118.234	C2—C3—C4	118.251	C2—C3—N4	123.718	C2—C3—N4	123.720
C3—C4—C4a	119.458	C3—C4—C4a	119.461	C3—N4—C4a	117.448	C3—N4—C4a	117.417
C4—C4a—C10b	118.593	C4—C4a—C10b	118.570	N4—C4a—C10b	123.257	N4—C4a—C10b	123.311
C4a—C10b—N1	120.302	C4a—C10b—N1	120.318	C4a—C10b—C1	117.303	C4a—C10b—C1	117.252
C10b—N1—C2	119.483	C10b—N1—C2	119.508	C10b—C1—C2	119.449	C10b—C1—C2	119.517
C4a—N5—C6	117.670	C4a—N5—C6	117.660	C4a—C5—N6	124.047	C4a—C5—N6	124.025
N5—C6—C6a	125.013	N5—C6—C6a	125.024	C5—N6—C6a	119.691	C5—N6—C6a	119.911
C6—C6a—C10a	119.326	C6—C6a—C10a	119.326	N6—C6a—C10a	121.781	N6—C6a—C10a	121.534
C6a—C10a—C10b	116.589	C6a—C10a—C10b	116.565	C6a—C10a—C10b	118.324	C6a—C10a—C10b	118.384
C10a—C10b—C4a	118.412	C10a—C10b—C4a	118.447	C10a—C10b—C4a	119.072	C10a—C10b—C4a	119.156
C10b—C4a—N5	122.984	C10b—C4a—N5	122.970	C10b—C4a—C5	117.082	C10b—C4a—C5	116.991
C6a—C7—C8	119.581	C6a—C7—C8	119.573	C6a—C7—C8	118.509	C6a—C7—C8	118.438
C7—C8—C9	120.249	C7—C8—C9	120.245	C7—C8—C9	121.116	C7—C8—C9	120.973
C8—C9—C10	121.670	C8—C9—C10	121.691	C8—C9—C10	120.929	C8—C9—C10	121.233
C9—C10—C10a	118.795	C9—C10—C10a	118.768	C9—C10—C10a	120.384	C9—C10—C10a	120.233
C10—C10a—C6a	117.791	C10—C10a—C6a	117.802	C10—C10a—C6a	119.794	C10—C10a—C6a	119.856
C10a—C6a—C7	121.912	C10a—C6a—C7	121.918	C10a—C6a—C7	119.254	C10a—C6a—C7	119.266
C9—C10—N11	119.550	C9—C10—N11	119.560	C6a—C7—N11	120.298	C6a—C7—N11	119.114
C10—N11—C12	126.290	C10—N11—C12	125.937	C7—N11—C12	125.861	C7—N11—C12	127.302
N11—C12—O13	123.419	N11—C12—O13	123.298	N11—C12—O13	117.222	N11—C12—O13	123.402
N11—C12—C14	115.707	N11—C12—C14	115.884	N11—C12—C14	121.492	N11—C12—C14	115.624
		C12—C14—C15	122.092			C12—C14—C15	121.885
		C14—C15—C16	119.749			C14—C15—C16	119.724
		C15—C16—C17	120.214			C15—C16—C17	120.200
		C16—C17—C18	120.023			C16—C17—C18	120.040
		C17—C18—C19	120.082			C17—C18—C19	120.084
		C18—C19—C14	119.873			C18—C19—C14	119.837
		C19—C14—C15	120.054				

The results have been obtained on a double Pentium III 733 MHz computer using Hyper Chem 4.5 program [18].

Aminodaps IV–VI have been obtained by reduction of corresponding nitrodaps [19], while acylaminodaps VII, IX by acetylation and VIII, X by benzylation of aminodaps [11, 20].

CONCLUSION

Correlations of experimental and calculated by the AM1 method wavenumber values of IV–X show good compatibility. Comparing r values for correlations of experimental and calculated by the AM1 and PPP methods wavenumber values of IV–VI, only slight differences have been found.

In the analysis of total energies of IV–VI calculated by the AM1, STO-3G, and 6-31G methods it was found that the values obtained by the first method are considerably higher than those obtained by other methods, which are comparable.

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