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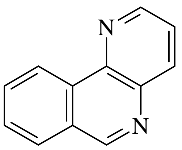
# UV spectral analysis of N- and C- substituted diazaphenanthrenes

**Abstract:** In the work the UV spectra of N- and C- substituted diazaphenanthrenes are presented along with comparison to spectra of parent 1,5-, 1,6- and 4,6-diazaphenanthrenes. The UV spectral values of considered compounds have been calculated by AM1 method and the correlation of experimental and calculated wavenumber values has been made.

**Keywords:** correlation, diazaphenanthrene, UV spectrum, wavenumber

## Introduction

Diazaphenanthrenes (dap) are heterocycles interesting so for their reactivity as well as due to their promising biological properties. In our study 1,5- , 1,6- and 4,6-daps **1- 3** are considered along with their N-derivatives **4-9** and C-derivatives **10 – 13**.



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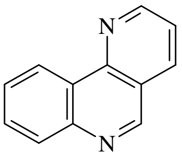

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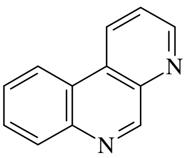

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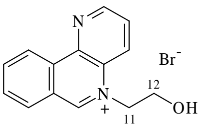
Among reactions of daps one should mention their quaternization and N-oxidation leading to N-substituted derivatives – quaternary salts [1-3] and N-oxides [4,5]. Some quaternary salts of daps are precursors of ylides used as 1,3-dipoles in cycloaddition reactions [6,7]. Due to the presence of nitrogen atoms, daps can form complexes with transition metal ions [8].

Daps undergo nitration affording C-substituted derivatives – nitrodaps, which upon reduction yield aminodaps, converted by diazotization and subsequent coupling reactions into dyes [9]. Aminodaps are synthons of tetracyclic compounds formed in Skraup procedure [10]. One should note also reactions of methyldaps, leading to corresponding aldehydes [11] or hydroxyethyldaps [12].

Correlations of experimental and calculated UV spectral values for dap derivatives substituted with nitro [13], formyl [14], methyl [15, 16], and amino [17, 18] groups as well as for their quaternary salts [19-21] and N-oxides [22] have been reported. Some daps show antibacterial, antifungal and antineoplastic properties [23, 24] and influence the enzymic activities in plants [25].

One should point out that N-substituted derivatives of azaaromatics, *i.e.* quaternary salts of azaaromatics are today a topic of an intense investigation; these compounds are interesting as building blocks in supramolecular chemistry [26-31], as synthons in chemical reactions [32, 33], as NLO materials [34], as catalysts [35, 36], ionic liquids [37], hydrogels [38], surfactants [39-41] and DNA binding species [42-44]; porphyrins bearing quaternary units [45-47] as well as viologens [48-50] deserve also an attention.



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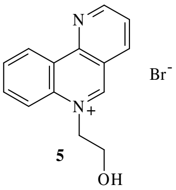

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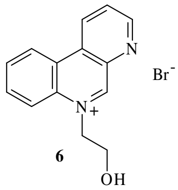

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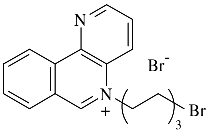
The present work is a continuation of our study concerning N- and C-substituted daps 4–13 [12]; its aim is the analysis of UV spectra of these compounds and correlation of their experimental and calculated wavenumber values.



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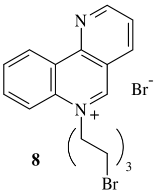

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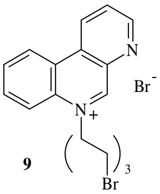

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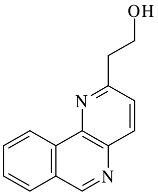

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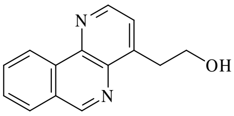

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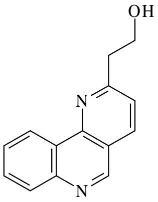

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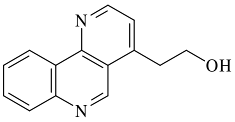

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## Experimental

The UV spectra have been recorded in 1,2-dichloroethane solution (c = $10^{-4}$M ) on a UV-Vis Specord spectrophotometer. Calculations were made by AM1 CI OC 35 method. The results have been obtained on a Pentium III 733 MHz computer with the use of Hyper Chem 4.5 program. N-Substituted daps **4–9** have been synthesized in quaternization reactions, and C-substituted daps **10–13** were obtained from corresponding methyldaps by treatment with formaldehyde [12].

## Results and Discussion

At first UV spectra of N-substituted, and then those of C-substituted daps will be shown. In Table 1 the UV spectra of N-substituted daps **4 – 9** are given, for comparative purposes spectra of parent daps **1- 3** [18] are included.

Table 1. Experimental $\overline{\nu}$ and log ε values of daps **1 – 3** [18] and of N-substituted daps **4 – 9**

| **Band** | $\overline{\nu}\cdot10^3$ cm$^{-1}$ | **log ε** | $\overline{\nu}\cdot10^3$ cm$^{-1}$ | **log ε** | $\overline{\nu}\cdot10^3$ cm$^{-1}$ | **log ε** |
|---|---|---|---|---|---|---|
| | **1** | | **2** | | **3** | |
| α | 27.6 | 3.750 | 29.1 | 3.114 | 29.0 | 3.211 |
| P | 38.1 | 4.245 | 38.2 | 4.376 | 38.1 | 4.342 |
| β | 42.2 | 4.519 | 43.6 | 4.472 | 43.3 | 4.451 |
| | **4** | | **5** | | **6** | |
| α | 31.4 | 3.875 | 26.0 | 3.190 | 29.7 | 3.000 |
| P | 36.7 | 4.204 | 31.0 | 3.169 | 38.0 | 3.613 |
| β | 41.5 | 4.728 | 36.2 | 3.663 | 41.3 | 3.767 |
| | **7** | | **8** | | **9** | |
| α | 25.0 | 3.477 | 25.3 | 3.982 | 25.3 | 3.964 |
| P | 32.2 | 3.672 | 30.2 | 4.000 | 32.1 | 4.140 |
| β | 36.2 | 3.989 | 35.3 | 4.441 | 35.6 | 4.481 |

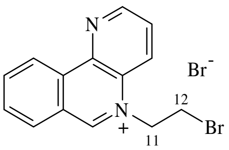
Comparing UV spectra of quaternary salts of daps with 2-bromoethanol, *i.e.* N-substituted daps **4–6** and those with 1,6-dibromohexane, *i.e.* N-substituted daps **7–9** it was observed that wavenumber values of α, p and β bands of **4–6** are higher than in the case of **7–9**.

Experimental UV spectra of N-substituted daps **4–9** have been compared with those of parent daps **1–3** [18]; the values of red and blue shifts are given in Table 2.

Table 2. Values of red and blue shifts of N-substituted daps **4–9** as compared with daps **1–3** [18] (positive values denote red, negative blue shifts)

| ***Band*** | **$\bar{\nu}$ Differences · $10^3$ (cm$^{-1}$)** | | |
|---|---|---|---|
| | **4/1** | **5/2** | **6/3** |
| $\alpha$ | -3.8 | +3.1 | -0.7 |
| P | +1.4 | +7.2 | +0.1 |
| $\beta$ | +0.7 | +7.4 | +2 |
| | **7/1** | **8/2** | **9/3** |
| $\alpha$ | +2.6 | +3.8 | +3.7 |
| P | +5.9 | +8 | +6 |
| $\beta$ | +6 | +8.3 | +7.7 |

Comparison of UV spectra of N-substituted daps **4–9** and those of quaternary salts of daps with 1,2-dibromoethane **14–16** [21] has been made; values of red and blue shifts are given in Table 3. All bands of **5** and **7–9** show the red shift, while for all bands of **4** and **6** the blue shift was observed.



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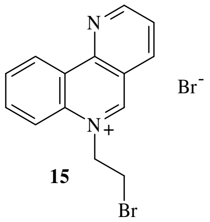

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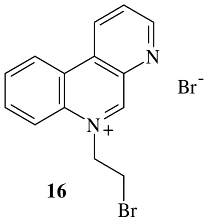

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Table 3. Values of red and blue shifts for N-substituted daps **4–9** as compared with those for quaternary salts of daps with 1,2-dibromoethane **14–16** [21].

| ***Band*** | **$\bar{\nu}$ Differences · $10^3$ (cm$^{-1}$)** | | |
|---|---|---|---|
| | **4/14** | **5/15** | **6/16** |
| $\alpha$ | -2.9 | +4.8 | -0.7 |
| p | -0.5 | +7 | -1 |
| $\beta$ | -0.7 | +5.8 | -0.7 |
| | **7/14** | **8/15** | **9/16** |
| $\alpha$ | +3.5 | +5.5 | +3.7 |
| p | +4 | +7.8 | +4.9 |
| $\beta$ | +4.6 | +6.7 | +6.4 |

In the analysis of UV spectra of C-substituted daps **10–13**, given in Table 4 it was observed that the wavenumber values of p and $\beta$ bands of compounds *para*-substituted relatively to nitrogen atom, *i.e.* **11** and **13** are higher than in the case of *ortho*-substituted compounds, *i.e.* **10** and **12**.

Table 4. Experimental $\bar{\nu}$ and log ε values of C-substituted daps **10–13**

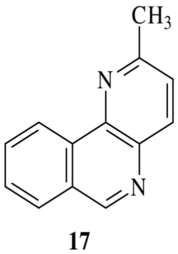
| | **10** | | **11** | | **12** | | **13** | |
|---|---|---|---|---|---|---|---|---|
| | **$\bar{\nu}\cdot 10^{3}\,\mathrm{cm}^{-1}$** | **log ε** | **$\bar{\nu}\cdot 10^{3}\,\mathrm{cm}^{-1}$** | **log ε** | **$\bar{\nu}\cdot 10^{3}\,\mathrm{cm}^{-1}$** | **log ε** | **$\bar{\nu}\cdot 10^{3}\,\mathrm{cm}^{-1}$** | **log ε** |
| α | 27.9 | 3.667 | 27.8 | 3.819 | 27.8 | 4.462 | 26.3 | 4.505 |
| P | 33.2 | 3.505 | 33.8 | 3.851 | 32.1 | 4.690 | 33.0 | 4.663 |
| β | 35.8 | 3.863 | 38.3 | 4.480 | 35.8 | 5.079 | 36.3 | 5.152 |

Experimental UV spectra of C-substituted daps **10–13** have been compared with those of corresponding daps **1** and **2** [18]; values of red and blue shifts are presented in Table 5. For all compounds the red shift was observed, except for α bands of **10** and **11** showing blue shift.

Table 5. Values of red and blue shifts of C-substituted daps **10–13** as compared with daps **1** and **2** [18]

| ***Band*** | **$\bar{\nu}$ Differences · $10^{3}$ ($\mathrm{cm}^{-1}$)** | | | |
|---|---|---|---|---|
| | **10/1** | **11/1** | **12/2** | **13/2** |
| α | -0.3 | -0.2 | +1.3 | +2.8 |
| P | +4.9 | +4.3 | +6.1 | +5.2 |
| β | +6.4 | +3.9 | +7.8 | +7.3 |

The UV spectra of C-substituted daps **10–13** have also been compared with spectra of corresponding methyldaps **17–20** [16]; values of red and blue shifts are given in Table 6. For all compounds the red shift was observed. For C-substituted daps **10–13**, the largest red shifts have been observed for **12** and **13**, so in comparison with parent daps **1** and **2** as well as in comparison with methyldaps **17–20**.



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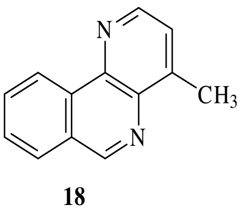

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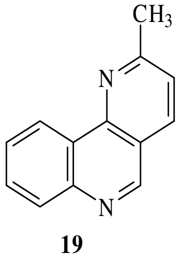

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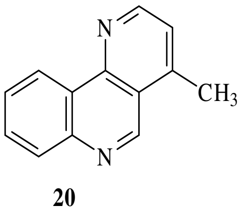

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Table 6. Values of red and blue shifts of C-substituted daps **10–13** as compared to those of methyldaps **17–20** [16]

| ***Band*** | **$\bar{\nu}$ Differences · $10^3$ ($cm^{-1}$)** | | | |
|---|---|---|---|---|
| | **10/17** | **11/18** | **12/19** | **13/20** |
| α | +1 | +1.3 | +2.8 | +4.1 |
| p | +4.3 | +4.2 | +5.9 | +5.4 |
| β | +5.6 | +1.7 | +7 | +5.8 |

Calculations concerning UV spectral values of N- and C-substituted daps have been made with semiempirical AM1 CI OC 35 method, which developed from MNDO procedure. The AM1 method is convenient for calculations of wavenumber and oscillator strength values of daps and their derivatives as compared with experimental data. This method is often used for azaaromatics, and is parametrized especially for these compounds.

Calculations of UV spectral values for N- and C-substituted daps **4–13** have been made using AM1 CI OC 35 method, next referred to as AM1; experimental data for these compounds along with calculated values are given in Tables 7–9.

Table 7. Experimental UV data with calculated bz AM1 method wavenumber and oscillator strength values for N-substituted daps **4-6**.

| | **4** | | | |
|---|---|---|---|---|
| | Experimental | | Calculated | |
| | $\bar{\nu} \cdot 10^3$ $cm^{-1}$ | log ε | $\bar{\nu} \cdot 10^3$ $cm^{-1}$ | f |
| α | 31.4 | 3.875 | 32.783 | 0.101 |
| p | 36.7 | 4.204 | 36.183 | 0.707 |
| β | 41.5 | 4.728 | 42.665 | 0.455 |
| | **5** | | | |
| | Experimental | | Calculated | |
| | $\bar{\nu} \cdot 10^3$ $cm^{-1}$ | log ε | $\bar{\nu} \cdot 10^3$ $cm^{-1}$ | f |
| α | 26.0 | 3.190 | 25.115 | 0.046 |
| p | 31.0 | 3.169 | 32.146 | 0.281 |
| β | 36.2 | 3.663 | 36.721 | 0.126 |
| | **6** | | | |
| | Experimental | | Calculated | |
| | $\bar{\nu} \cdot 10^3$ $cm^{-1}$ | log ε | $\bar{\nu} \cdot 10^3$ $cm^{-1}$ | f |
| α | 29.7 | 3.000 | 32.459 | 0.279 |
| p | 38.0 | 3.613 | 38.962 | 0.362 |
| β | 41.3 | 3.767 | 42.434 | 0.330 |

Table 8. Experimental UV data with calculated by AM1 method wavenumber and oscillator strength values for N-substituted daps **7-9**.

| | **7** | | | |
|---|---|---|---|---|
| | Experimental | | Calculated | |
| | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | log ε | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | f |
| α | 25.0 | 3.477 | 24.987 | 0.131 |
| p | 32.2 | 3.672 | 32.884 | 0.099 |
| β | 36.2 | 3.989 | 36.332 | 0.446 |
| | **8** | | | |
| | Experimental | | Calculated | |
| | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | log ε | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | f |
| α | 25.3 | 3.982 | 25.264 | 0.046 |
| p | 30.2 | 4.000 | 32.291 | 0.267 |
| β | 35.3 | 4.441 | 35.473 | 0.287 |
| | **9** | | | |
| | Experimental | | Calculated | |
| | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | log ε | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | f |
| α | 25.3 | 3.964 | 25.403 | 0.038 |
| p | 32.1 | 4.140 | 32.694 | 0.237 |
| β | 35.6 | 4.481 | 35.723 | 0.430 |

Table 9. Experimental UV data with calculated by AM1 method wavenumber and oscillator strength values for N-substituted daps **10-13**.

| | **10** | | | |
|---|---|---|---|---|
| | Experimental | | Calculated | |
| | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | log ε | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | f |
| α | 27.9 | 3.667 | 27.813 | 0.062 |
| p | 33.2 | 3.505 | 34.435 | 0.050 |
| β | 35.8 | 3.863 | 38.148 | 1.262 |
| | **11** | | | |
| | Experimental | | Calculated | |
| | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | log ε | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | f |
| α | 26.3 | 4.505 | 27.535 | 0.008 |
| p | 33.0 | 4.663 | 33.112 | 0.024 |
| β | 36.3 | 5.152 | 37.083 | 1.124 |
| | **12** | | | |
| | Experimental | | Calculated | |
| | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | log ε | $\bar{\nu} \cdot 10^{3}$ cm$^{-1}$ | f |
| α | 27.8 | 4.462 | 27.474 | 0.013 |
| p | 32.1 | 4.690 | 33.136 | 0.023 |
| β | 35.8 | 5.079 | 37.027 | 1.147 |

Table 9. cont.

| | **13** | | | |
|---|---|---|---|---|
| | Experimental | | Calculated | |
| | $\bar{\nu} \cdot 10^3$ cm$^{-1}$ | log ε | $\bar{\nu} \cdot 10^3$ cm$^{-1}$ | f |
| α | 26.3 | 4.505 | 27.535 | 0.008 |
| p | 33.0 | 4.663 | 33.112 | 0.024 |
| β | 36.3 | 5.152 | 37.083 | 1.124 |

For N- and C-substituted daps **4–13** correlations of experimental and calculated wavenumber values have been made.

Correlations of experimental and calculated by AM1 method wavenumber values for N-substituted daps **4–9** are:

| **for 4–6** | **for 7–9** |
|---|---|
| a = 1.017; b = 0.277; r = 0.963 | a = 1.013; b = 0.019; r = 0.980 |

Comparison of correlation coefficients for these both groups of compounds shows for **7–9** higher r than for **4–6**.

The correlations of experimental and calculated wavenumber values for **4–6** and **7–9** with corresponding parent daps **1–3** are:

for 4/1 a = 0.983; b = 1.958; r = 0.969
for 5/2 a = 1.039; b = 1.138; r = 0.985
for 6/3 a =0.959; b =2.545; r = 0.969
for 7/1 a = 1.065; b = -1.046; r = 0.983
for 8/2 a = 0.986; b = 0.858; r = 0.978
for 9/3 a = 1.035; b = - 0.809; r = 0.993

In the above correlations, for **4–6** the highest r value is in the case of **5/2** (r=0.985), and for **7–9** the highest r value is in the case of **9/3** (r= 0.993).

Correlations of experimental and calculated by AM1 method wavenumber values for C-substituted daps **10–13** are :

| **for 10 and 11** | **for 12 and 13** |
|---|---|
| a = 1.075; b = -1.821; r = 0.956 | a = 1.036; b = -0.480; r = 0.979 |

Comparing the above results, for **10** and **11**, which are derivatives of dap **1** the correlation coefficient is lower (r= 0.956) than for **12** and **13**, which are derivatives of dap **2** (r=0.979).

The correlations of experimental and calculated wavenumber values for **10**, **11** and **12**, **13** with corresponding parent daps **1**, **2** are:

| | |
|---|---|
| for 10/1 | a = 1.087; b = -1.415; r = 0.983 |
| for 11/1 | a = 1.030; b = 0.033; r = 0.969 |
| for 12/2 | a = 1.026; b = -0.538; r = 0.983 |
| for 13/2 | a = 0.975; b = 1.275; r = 0.987 |

In the above correlations, for **10**, **11** the higher r value is in the case of **10/1** (r=0.983), and for **12**, **13** the higher r value is in the case of **13/2** (r=0.987).

## Conclusion

In correlations of experimental and calculated by AM1 method wavenumber values for N- and C-substituted daps **4–13**, higher correlation coefficients have been obtained for N-substituted daps **7–9**, *i.e.* quaternary salts of daps with 1,6-dibromohexane than for **4–6**, *i.e.* quaternary salts of daps with 2-bromoethanol.

## References

1. W. Śliwa, *Current Org. Chem.* 2003, **7**, 995.
2. B. Bachowska, T. Zujewska, *ARKIVOC*, 2001, ***Part VI***, 77.
3. B. Dondela, W. Śliwa, *Khim. Get. Soedin.,* 2000, 944.
4. T. Zujewska, B. Bachowska, *Polish J. Chem.* 1998, **72**, 2507.
5. T. Zujewska, B. Bachowska, *Aust. J. Chem.* 1996, **49**, 523.
6. G. Matusiak, *Aust. J. Chem.* 1999, **52**, 149.
7. B. Bachowska, T. Zujewska, *Polish J. Chem.* 1996, **70**, 1324.
8. A. Gaudyn, W. Śliwa, *Chem. Papers* 1994, **48**, 306.
9. L. Chrząstek, W. Śliwa, *Chem. Papers* 2001, **55**, 42.
10. W. Śliwa, M. Mielniczak, *Chem. Papers* 1998, **52**, 747.
11. L. Chrząstek, B. Mianowska, W. Śliwa, *Aust. J. Chem.* 1994, **47**, 2129.
12. M. Deska, W. Śliwa, *Chem. Papers* 2002, **56**, 309.
13. J. Peszke, L. Chrząstek, W. Śliwa, *Prace Naukowe WSP w Częstochowie, (Pedagogical University Issues)*, Chemia VII, Częstochowa 2003, 63.
14. J. Peszke, B. Mianowska, W. Śliwa, *Spectrochim. Acta* 1997, **53A**, 2565.
15. B. Mianowska, W. Śliwa, *Spectrochim. Acta* 1996, **52A**, 397.
16. B. Mianowska, W. Śliwa, *Acta Chim. Hung. Models Chem.* 1994, **131**,761.
17. J. Peszke, L. Chrząstek, W. Śliwa, *Chem. Papers* 2004, **58**, 176.
18. B. Mianowska, W. Śliwa, *Acta Chim. Hung.* 1991, **128**, 93.
19. B. Dondela, J. Peszke, W. Śliwa, *J. Mol. Struct.* 2005, **753**, 154.
20. J. Peszke, W. Śliwa, *Spectrochim. Acta* 2002, **58A**, 2127.

21. J. Peszke, M. Mielniczak, W. Śliwa, *Prace Naukowe WSP w Częstochowie, (Pedagogical University Issues)*, Chemia II, Częstochowa 1998, 145.
22. J. Peszke, W. Śliwa, *Prace Naukowe WSP w Częstochowie, (Pedagogical University Issues)*, Chemia IV, Częstochowa 1999, 145.
23. L. Chrząstek, M. Mielniczak, Z. Staroniewicz, W. Śliwa, *Khim. Get. Soedin.* 1999,1396.
24. R. Kovačič, M.A. Kassel, J.R. Ames, B.A. Feinberg, W. Śliwa, *J. Biopharm. Sci.* 1990, **1**, 331.
25. E. Gurgul, B. Herman, R. Biczak, W. Śliwa, *Sci. Agric. Bohem.* 1997, **28**, 245.
26. T. D. Nguyen, H.-R. Tseng, P.C. Celestre, A.H. Flood, Y. Liu, J.F. Stoddart, J. I. Zink, *Proceed. Natl. Acad. Sci. USA* 2005, **102**, 10029.
27. Y. Liu, A.H. Flood, P.A. Bonvallet, S.A. Vignon, B.H. Northrop, H.-R. Tseng, J.O. Jeppesen, T. J. Huang, B. Brough, M. Baller, S. Magonov, S.D. Solares, W. A. Goddard, Ch.-M. Ho, J.F. Stoddart, *J. Am. Chem. Soc.* 2005, **127**, 9745.
28. M. Ceccarelli, F. Mercuri, D. Passerone, M. Parrinello, *J. Phys. Chem.* 2005, **109B**, 17094.
29. Y. Liu, S.A. Vignon, X. Zhang, K.N. Houk, J.F. Stoddart, *Chem. Commun.* 2005, 3927.
30. W. Śliwa, T. Zujewska, *Heterocycles*, 2005, **65**, 1713.
31. W. Śliwa, B. Bachowska, *Heterocycles*, 2004, **63**, 2131.
32. X. Feng, E. N. Duesler, P. S. Mariano, *J. Org. Chem.* 2005, **70**, 5618.
33. E. Chrobak, A. Maślankiewicz, *Heterocycles* 2004, **63**, 2329.
34. B.J. Coe, D. Beljonne, H. Vogel, J.J. Garin, J. Orduna, *J. Phys. Chem.* 2005, **109A**, 10052.
35. T. Maki, K. Ishihara, H. Yamamoto, *Org. Lett.* 2005, **7**, 5047.
36. K. Suga, K. Ohkubo, S. Fukuzumi, *J. Phys. Chem.* 2005, **109A**, 10168.
37. A. Taubert, P. Steiner, A. Mantion, *J. Phys. Chem.* 2005, **109B**, 15542.
38. M. Suzuki, M. Yumoto, H. Shirai, K. Hanabusa, *Org. Biomol. Chem.* 2005, **3**, 3073.
39. M. Almgren, V. M. Garamus, *J. Phys. Chem.* 2005, **109B**, 11348.
40. Y. Yang, M. Suzuki, S. Owa, H. Shirai, K. Hanabusa, *Chem. Commun.* 2005, 4462.
41. T. Chakraborty, S. Ghosh, S. Moulik, *J. Phys. Chem.* 2005, **109B**, 14813.
42. L. Valis, N. Amann, H.-A. Wagenknecht, *Org. Biomol. Chem.* 2005, **3**, 36.
43. N.W. Luedtke, Q. Liu, Y. Tor, *Chem. Eur. J.* 2005, **11**, 495.
44. N. Morii, G. Kido, T. Konakahara, H. Morii, *J. Phys. Chem.* 2005, **109B**, 15636.
45. A. Brisach-Wittmeyer, S. Lobstein, M. Gross, A. Giraudeau, *J. Electroanal. Chem.* 2005, **576**, 129.
46. M. Balaz, M. De Napoli, A.E. Holmes, A. Mammana, K. Nakanishi, N. Berova, R. Purrello, *Angew. Chem. Int. Ed.* 2005, **44**, 4006.
47. J. Kang, H. Wu, X. Lu, Y. Wang, L. Zhou, *Spectrochim. Acta.* 2005, **61A**, 2041.
48. V. Balzani, P. Ceroni, C. Giansante, V. Vicinelli, F.-G. Klärner, C. Verhaelen, F. Vögtle, U. Hahn, *Angew. Chem. Int. Ed.* 2005, **44**, 4574.
49. F. Huang, K.A. Switek, H.W. Gibson, *Chem. Commun.* 2005, 3655.
50. J.W. Park, S.Y. Lee, H.J. Song, K.K. Park, *J. Org. Chem.* 2005, **70**, 9505.

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# Analiza widm UV N- i C-podstawionych diazafenantrenów

**Streszczenie:** W pracy przedstawiono widma UV N- i C-podstawionych diazafenantrenów oraz porównano je z widmami niepodstawionych diazafenantrenów. Stosując metodę AM1 obliczono wartości dotyczące widm UV dla rozważanych związków oraz przeprowadzono korelacje doświadczalnych i obliczonych wartości ich liczb falowych.

**Słowa kluczowe:** diazafenantren, korelacja, liczba falowa, widmo UV