Journal of Molecular Structure 1027 (2012) 116–123

Contents lists available at SciVerse ScienceDirect

Journal of Molecular Structure

journal homepage: www.elsevier.com/locate/molstruc

Pyridylmethylsilanes as dicarboxyacid receptors: Experimental and theoretical study

Bogusława Łęska *, Grzegorz Schroeder, Radosław Pankiewicz, Bogusława Mikisz

Faculty of Chemistry, A. Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland

HIGHLIGHTS

- A series of new Si-tripodal receptors, based on 1-3 pyridylmethyl was synthesized.
- All new compounds was characterized by ^{1}H and ^{13}C NMR.
- A new complexes between synthesised species and dicarboxyacid anions was obtained and studied by ^{19}F NMR.
- All supramolecular complexes were structurally authenticated using quantum-mechanical calculation.

ARTICLE INFO

Article history:
Received 18 April 2012
Received in revised form 25 May 2012
Accepted 26 May 2012
Available online 6 June 2012

Keywords:
Si-anion receptors
Anion recognition
Calculation
Theoretical methods

ABSTRACT

A series of literature known (**1–3**) [1–4] and new Si-tripodal receptors for anion sensing, based on 1–3 pyridylmethyl functionalized side arms as recognition sites, was designed, successfully synthesized and characterized by ^{1}H and ^{13}C NMR spectra (**4–9**). These ligands showed high selectivity and strong binding affinity toward investigated dicarboxyacid anions. The complexes formation was confirmed by ^{19}F NMR spectra.

All supramolecular complexes were structurally authenticated using parametric method 5 (PM5) with the MO-G for SCIGRESS program. The results brought information of the type and nature of intermolecular interactions present in the complexes and extended structures.

1. Introduction

For the last 40 years, dynamic and rapid development of supramolecular chemistry has been possible by expansion of many efficient methods of molecular receptors synthesis. The new strategies of their synthesis allow obtaining molecular receptors of specific properties and capabilities (host molecules) for selective recognition of complex molecules (guests). Podands make a group of open-chain analogs of macrocyclic compounds, such as crown ethers or cryptands. Because they can be easily synthesized and their synthesis is low cost, podands are useful in many areas of chemistry. The compounds of this class are able to form stable complexes with metal cations (alkali, alkaline earth or heavy metals), neutral molecules and also different types of anions [5–19].

The design and synthesis of receptors capable of selective binding and sensing cations and anions remains challenging and it is an area of active research. During the development of artificial receptor the selectivity, interactions between host and guest have to be considered in a complementary fashion. Several strategies can be followed in the design of unmaterial receptors with optimal selectivity toward a particular ion. The tripodal receptors make one of the most important and special classes of receptors with each arm bearing a functional group that can coordinate with the target ion [20–26].

The number of tripodal ligands for recognition of alkali and alkaline earth metal ions reported in literature is limited. Shanzer and co-workers [27] used tripodal structures with flexible arms, based on trimethylolpropane, for the complexation of Ca^{2+}. We have also shown that the silicon and phosphorous podands form stable complexes with silver (I) cations of various stoichiometry depending on the length of the oxaalkyl chains [28,29].

The significance of anion recognition has grown because anions play important roles in chemical and biochemical processes, some of which are also of great environmental and medical concern. In comparison with the podand cation complexes, the formation of podand anion complexes is a relatively new field still poorly explored. Literature gives a lot of papers devoted to ligands complexing anions. In the years 2000–2012 almost 4700 scientific reports on anion synthetic receptors were published, but usually there

* Corresponding author.
E-mail address: bogunial@amu.edu.pl (B. Łęska).

0022-2860/$ - see front matter © 2012 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.molstruc.2012.05.069

were notes about a few systems of cyclic (polimacrocyclic) ligands, such as pyrrols, amides, urea (thiourea) moieties, polyammonium(guanidiniums), Lewis acids, calix[n]arenas [12–19,30–39], while only a few were related to podands that are able to complex anions [25,40–44].

Most hydrogen bonding anion (**A**) receptors are based on N–H–**A** or O–H–**A** hydrogen bonds, while C–H–**A** hydrogen bonds are rarely utilized for anion binding even though C–H hydrogen bond plays an important role in nature [42,45–47]. For example, the urea functional group, well-known for its ability to interact with anions through hydrogen bonds interactions, was chosen as a scaffold for the construction of combined hydrogen/halogen bonding receptors. The urea (thiourea) moieties are particularly good hydrogen bond donors and are excellent receptors for anions such as phosphate via the formation of two hydrogen bonds [35].

Polyammonium (guanidinium) are also known to be compatible with biological systems [48–50] and their lipid bilayer transport properties are comparable to those of simple thiourea. For instance, P.A. Gale and co-workers have demonstrated that thiourea isosteres such as functionalized cyanoguanidines and the hexyl derivative of 3-amino-1,2,4-benzothiadiazine-1,1-dioxide are capable of binding and transporting anions [36].

Anions are relatively large and therefore require receptors much larger than cations. Moreover, their specific properties resulting from their spatial structure and the size of ionic radius make them highly sensitive to the environmental (pH), etc. Furthermore, in comparison with similar size cations, anions are characterized by higher values of free energy barrier, therefore, the receptors, that would complex anions must overcome a significant energy barrier, as a result of environmental impacts on the reaction. Even a small change in pH value of the environment of given anions, could result in a loss of anions charge by proton attachment.

The aim of our study was to synthesize podand complexes with three selected acids and characterize them by ^{13}C and ^{19}F NMR methods. The results were interpreted in confrontation with the outcome of calculations by PM5 method. We have successfully synthesized new podand receptors capable of binding dicarboxylic acids (anions) by hydrogen bonds to make complexes of different stoichiometry and structure.

2. Experimental section

2.1. Used reagents

All products: 2-pyridinemethanol, 3-pyridinemethanol, 4-pyridinemethanol, triethylamine, chlorotrimethylsilane, dichloromethyl-octadecylsilane, trichloro(methyl)silane, tetrafluorophtalic acids, such as tetrafluorophthalic acid (**DKFBo**), tetrafluoroisophthalic acid (**DKFBm**), tetrafluoroterephthalic acid (**DKFBp**), used for the synthesis of silanes and complexes, were purchased from Aldrich and were used without purification. The solvents (tetrahydrofuran, ethyl ether, acetonitrile, chloroform) and magnesium sulfate were also used as commercial products (Aldrich).

2.2. Synthesis silanes

2.2.1. Synthesis of monopyridylsilanes: 2-pyridyl-methylenoxytrimethylsilane (1), 3-pyridyl-methylenoxytrimethylsilane (2), 4-pyridyl-methylenoxytrimethylsilane (3)

Monopyridylsilane receptors (**1–3**) were readily synthesized as a yellow oils from the reaction of the appropriate 2-, 3- or 4-pyridinemethanol with chlorotrimethylsilane (molar ratio = 1:1). To a tetrahydrofuran (THF) (200 mL) solution of 24.9 g of appropriate pyridinemethanol at room temperature, triethylamine was added (32.7 mL). Then 24.9 mL chlorotrimethylsilane was added dropwise. The mixture was stirred under reflux at room temperature for 22 h. The consumption of the starting material was confirmed by TLC analysis.

After this time the obtained product was filtered off using a Büchner funel. The solvent was evaporated in a vacuum evaporator and the residue was extracted with ethyl ether (150 mL) and water (2×75 mL). The organic layer was separated, dried over magnesium sulfate, decanted and again evaporated in vacuum evaporator to give yellow oil products (**1–3**) (Table 1). The products were identified by ^{1}H and ^{13}C NMR methods and their purity was estimated (Tables 4 and 5).

2.2.2. Synthesis of dipyridylsilanes – di(2-pyridyl-methylenoxy)methylooctadecylsilane (4), di(3-pyridyl-methylenoxy)methylooctadecylsilane (5), di(4-pyridyl-methylenoxy)methylooctadecylsilane (6)

Dipyridylsilane receptors (**4–6**) were synthesized as a yellow oils from the reaction of the appropriate 2-, 3- or 4-pyridinemethanol with dichloro-methyl-octadecylsilane (molar ratio = 2:1). To a tetrahydrofuran (THF) (250 mL) solution of 10 g pyridinemethanol at room temperature, triethylamine (12.8 mL) was added. Then 12.8 mL dichloro-methyl-octadecylsilane was added dropwise. The mixture was stirred under reflux at room temperature for 22 h. The consumption of the starting material was confirmed by TLC analysis.

After this time the obtained product was filtered off using a Büchner funel. The solvent was evaporated in a vacuum evaporator and the residue was extracted with ethyl ether (150 mL) and water (2×75 mL). The organic layer was separated, dried over magnesium sulfate, decanted and again evaporated in vacuum evaporator to give yellow oil products (**4–6**) (Table 2). The products were identified by ^{1}H and ^{13}C NMR methods and their purities were estimated (Tables 4 and 5).

2.2.3. Synthesis of trispyridylmethoxysilanes – tris(2-pyridylmethylenoxy)methyl silane (7), tris(3-pyridyl-methylenoxy)methyl silane (8), tris(4-pyridyl-methylenoxy)methylsilane (9)

Trispyridylmethoxysilanes receptors (**7–9**) were synthesized in reactions of the appropriate 2-, 3- or 4-pyridinemethanol with trichloromethylsilane (molar ratio = 3:1). To a tetrahydrofuran (THF) (200 mL) solution of 17 g pyridine at room temperature triethylamine (22 mL) was added. Then 6.1 mL trichloromethylsilane was added dropwise. The mixture was stirred under reflux at room temperature for 22 h. The consumption of the starting material was confirmed by TLC analysis.

After this time the product obtained was filtered off using a vacuum Erlenmeyer flask connected to a vacuum pump. The solvent was evaporated in a vacuum evaporator and the residue was extracted with diethyl ether (150 mL) and water (2×75 mL). The organic layer was separated, dried over $MgSO_4$, decanted and again evaporated in a vacuum evaporator to obtain the solid (gelatinous) or liquid product (**7–9**) (Table 3). The products were identified ^{1}H and ^{13}C NMR methods and their purities were estimated (Tables 4 and 5).

2.3. NMR studies

The NMR spectra were recorded in CD_3CN using a Varian Gemini 300 MHz spectrometer. All spectra were locked to deuterium resonance of CD_3CN and $CDCl_3$. The error in ppm values was 0.01.

All ^{1}H NMR measurements of the silanes obtained were carried out at the operating frequency sfrq = 300.069 MHz; flip angle, pw = 8.8 μs; spectral width, *sw* = 4500 Hz; acquisition time, *at* = 3–3.5 s; relaxation delay, *d*1 = 0–1.0 s; *T* = 293.0 K and TMS as the internal standard. No window function or zero filling was used.

Table 1
The yields and characteristic of monopyridylsilanes.

Name	Structure	Yield (%)
2-pyridyl-	methylenoxytrimethylsilane (**1**)	40
3-pyridyl-	methylenoxytrimethylsilane (**2**),	48
4-pyridyl-	methylenoxytrimethylsilane (**3**)	60

Table 2
The yields and characteristic of dipyridylsilanes.

Name	Structure	Yield (%)
di(2-pyridylmethylenoxy) methyloctadecylosilane (**4**)		50
di(3-pyridylmethylenoxy) methyloctadecylosilane (**5**)		46
di(4-pyridylmethylenoxy) methyloctadecylosilane (**6**)		55

Digital resolution was 0.2 Hz/point. The data obtained are collected in Table 4.

^{13}C NMR spectra of the silanes obtained were recorded at the operating frequency sfrq = 75.459 MHz; *pw* = 9.3 μs; *sw* = 22573.4 Hz; *at* = 1.5 s; *d*1 = 0 s; *T* = 293.0 K and TMS as the internal standard. Line broadening parameters were 0.5 or 1 Hz. The data obtained are collected in Table 5.

Table 3
The yields and characteristic of trispyridylmethoxysilanes.

Name	Structure	Yield (%)
tris(2-pyridylmethylenoxy) methylsilane (**7**)		58
tris(3-pyridylmethylenoxy) methylsilane (**8**)		47
tris(4-pyridylmethylenoxy) methylsilane (**9**)		63

The complexes formation between silanes and tetrafluoric acid (stoichiometry 1:1) was verified by ^{19}F NMR. The ^{19}F NMR spectra were recorded at the operating frequency sfrq = 282.319 MHz; *at* = 0.71 s; *sw* = 90090.1 Hz; *pw* = 5.0 μs; *d*1 = 1 s; *T* = 293.0 K and TMS as the internal standard. Line broadening parameters were 0.5 or 1 Hz.

2.4. Theoretical calculation

All semi-empirical calculations for the complexes (adducts) between the ligands obtained and tetrafluorophtalic, acids were performed using the Win Mopac 2007 parametric method 5 (PM5) with the MO-G for SCIGRESS program [51]. All initial structures were optimized at first by the molecular mechanics method

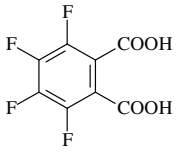
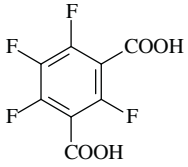
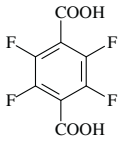
Table 4
Chemical shifts ^{1}H NMR for obtained receptors in CD_3CN (293 K) (ppm).

Ligand	H2	H3	H4	H5	H6	H7	H8	H9 (Si–CH_2)	–$(CH_2)_{16}$–	Me ($C_{18}H_{37}$)
1	–	7.342 (d)	7.504 (t)	6.958 (t)	8.341 (d)	4.661 (s)	0.034 (s)	–	–	–
2	8.379 (s)	–	7.440 (d)	7.042 (t)	8.302 (d)	4.507 (s)	0.055 (s)	–	–	–
3	8.544 (d)	7.264 (d)	–	7.264 (d)	8.544 (d)	4.706 (s)	0.176 (d)		–	–
4	–	7.498 (d)	7.677 (t)	7.260 (t)	8.495 (t)	4.911 (s)	0.243 (s)	0.739 (t)	1.245–1.423 (m)	0.869 (s)
5	8.543 (s)	–	7.609 (d)	7.260 (t)	8.501 (d)	4.767 (s)	0.201 (s)	0.678 (t)	1.245–1.424 (m)	0.870 (s)
6	8.523 (d)	7.223 (d)	–	7.223 (d)	8.523 (d)	4.767 (s)	0.218 (s)	0.704 (t)	1.236–1.415 (m)	0.861 (s)
7	–	7.297 (d)	7.650 (t)	7.166 (t)	8.488 (d)	4.739 (s)	0.202 (s)	–	–	–
8	8.489 (s)	–	7.691 (d)	7.259 (t)	8.433 (d)	4.687 (s)	0.195 (s)	–	–	–
9	8.500 (d)	7.188 (d)	–	7.188 (d)	8.500 (d)	4.828 (s)	0.238 (s)	–	–	–

Table 5
Chemical shifts ^{13}C NMR for obtained receptors in CD_3CN (293 K) (ppm).

Ligand	C2	C3	C4	C5	C6	C7	C8	C9 (Si–CH_2)	–$(CH_2)_{16}$–	Me ($C_{18}H_{37}$)
1	160.578	119.839	136.146	121.464	148.353	65.240	−0.890	–	–	–
2	147.837	135.739	133.676	122.715	147.837	61.684	−0.995	–	–	–
3	150.441	121.777	151.409	121.777	150.441	63.540	−0.650	–	–	–
4	160.286	121.998	136.876	120.223	148.481	65.313	−2.716	−4.880	14.093–33.198 (m)	13.709
5	148.732	135.685	134.219	123.277	148.732	62.186	−2.995	−4.793	14.097–33.179 (m)	13.695
6	149.585	120.693	149.585	120.693	149.585	62.839	−2.642	−4.935	14.079–33.874 (m)	13.563
7	159.423	122.236	136.236	120.629	148.339	64.154	−4.624	–	–	–
8	148.321	136.853	134.995	123.509	148.111	62.159	−5.898	–	–	–
9	149.681	120.647	148.640	120.647	149.681	63.104	−4.688	–	–	–

Table 6
Chemical shifts ^{19}F NMR for tetrafluorophtalic acids and obtained complexes (ligands with tetrafluorophtalic acids) in CD_3CN.

Chemical shifts (Δ of chemical shifts; complex – free acid) ^{19}F NMR										
Tetrafluorophtalic acids $C_8H_4F_40_4$	Complexes tetrafluorophtalic acids and ligands									
	Acid + ligand 1	Acid + ligand 2_4	Acid + ligand 3	Acid + ligand 4	Acid + ligand 5	Acid + ligand 6	Acid + ligand 7	Acid + ligand 8	Acid + ligand 9	
DKFBo 	−138.061	−140.821 (−2.760)	−140.841 (−2.780)	−140.994 (−2.933)	−141.528 (−3.467)	−141.290 (−3.229)	−141.354 (−3.293)	−141.240 (−3.179)	−141.211 (−3.150)	−141.342 (−3.281)
	−150.742	−154.400 (−3.658)	−154.413 (−3.671)	−154.690 (−3.948)	−155.671 (−4.929)	−154.989 (−4.247)	−155.033 (−4.291)	−154.880 (−4.138)	−154.734 (−3.992)	−155.128 (−4.386)
DKFBm 	−113.308	−117.147 (−3.839)	−118.177 (−4.869)	−118.123 (−4.815)	−116.523 (−3.215)	−117.845 (−4.537)	−117.965 (−4.657)	−116.394 (−3.086)	−117.719 (−4.411)	−118.005 (−4.697)
	−127.557	−133.165 (−5.608)	−134.387 (−6.830)	−134.324 (−6.767)	−133.192 (−5.635)	−133.27 (−5.713)	−134.241 (−6.684)	−132.852 (−5.295)	−133.784 (−6.227)	−134.057 (−6.500)
DKFBp 	−162.969	−164.491 (−1.522)	−164.637 (−1.668)	−164.678 (−1.709)	−164.150 (−1.181)	−164.145 (−1.176)	−164.097 (−1.128)	−163.810 (−0.841)	−164.001 (−1.032)	−164.354 (−1.385)
	−139.154	−142.070 (−2.916)	−141.401 (−2.247)	−142.359 (−3.205)	−142.239 (−3.085)	−141.323 (−2.169)	−141.916 (−2.762)	−142.085 (−2.931)	−141.135 (−1.981)	−142.039 (−2.885)

(MM2). In all cases full geometry optimization was carried out without any symmetry constraints. The bonding energies (E) (kJ/mol) between F-acid and silanes were calculated as differences between the heat of formation (HOF) of the acid and silane with a hydrogen bond and the sum of HOFs of isolated species.

3. Results and discussion

Molecular recognition of systems can be achieved thanks to the specific character of the interactions between the receptor and the guest molecules, which may involve ionic bonds, dipole interactions,

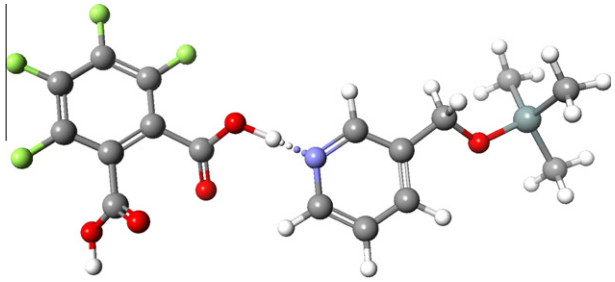


Fig. 1. Calculated (PM5) structure of DKFBo with ligand (2) with one hydrogen bond.

Table 7
The theoretical parameters interaction between silane ligands and tetrafluorophtalic acids.

Tetrafluorophtalic acids	Symbol of adduct	The length of hydrogen bond (Å)	Number of hydrogen bonds	ΔHOF (kJ/mol)*
DKFBo				
	DKFBo + 2	2.433	1	−65.43
	DKFBo + 5	2.505	1	−52.17
	DKFBo + 5	2.582	2	−89.00
		2.586		
	DKFBo + 8	2.504	1	−51.03
	DKFBo + 8	2.569	2	−89.96
		2.573		
DKFBm				
	DKFBm + 2	2.687	1	−55.86
	DKFBm + 5	2.514	1	−49.82
	DKFBm + 5	2.779	2	−44.51
		2.784		
	DKFBm + 8	2.610	1	−40.90
	DKFBm + 8	2.799	2	−29.10
		2.802		
DKFBp				
	DKFBp + 2	2.565	1	−56.03
	DKFBp + 5	2.622	1	−52.72
	DKFBp + 5	2.767	2	−45.18
		2.770		
	DKFBp + 8	2.533	1	−57.07
	DKFBp + 8	2.744	2	−38.89
		2.748		

$\Delta HOF = HOF_{A\cdots H\cdots B} - HOF_{AH+B}$ or $\Delta HOF = HOF_{H\overset{B}{\underset{A}{\cdots}}H} - HOF_{HAH+B}$.

van der Waals forces or hydrogen bonds. When the recognition takes place with formation of a hydrogen bond, of major importance are its geometry (bond angle) and length. In the molecular receptors in which hydrogen bonds determine the selectivity of interactions, the structures of the receptor and the guest plays a crucial role.

A series of nine new pyridylmethyl Si-podand receptors (1–9) was obtained. These potential receptors contained from three to nine free electron pairs (pyridine nitrogen atom) able to form hydrogen bonds in complexes with dicarboxylic acids (HAH).

The structure of dicarboxylic acids and pyridylmethyl Si-podand determine molecular recognition and thus the selectivity of the newly obtained molecular receptors. The nature of the receptor–anion interactions was characterized by ^{19}F NMR experiment. The chemical shift of ^{19}F NMR was used as probe of selective molecular recognition.

Three fluoric acids, characterized by different (orto, meta and para) arrangements of carboxyl groups in perfluoroaromatic rings were selected. The data obtained are collected in Table 6.

For all systems studied addition of equimolar amounts of pyridylmethyl Si-podands caused changes in the chemical shift values of fluorine atoms in fluorodicarboxylic acids observed in the ^{19}F NMR spectra. The value change is comparable in size for all

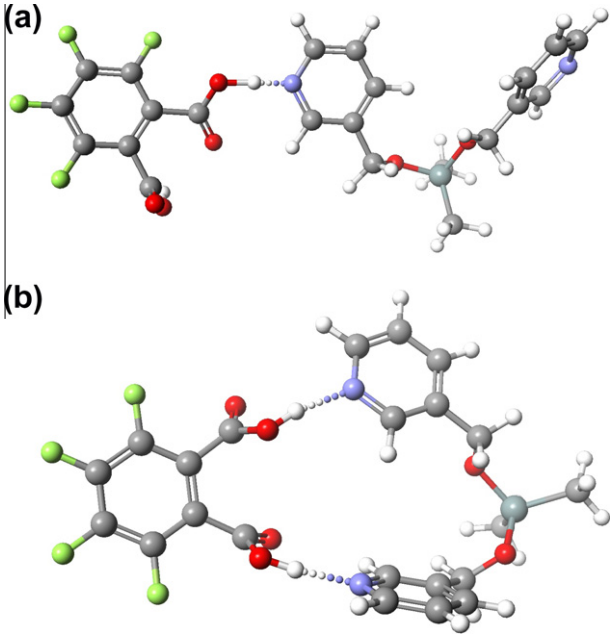


Fig. 2. Calculated (PM5) structure of DKFBo with ligand (5): (a) with one hydrogen bond and (b) with two hydrogen bonds.

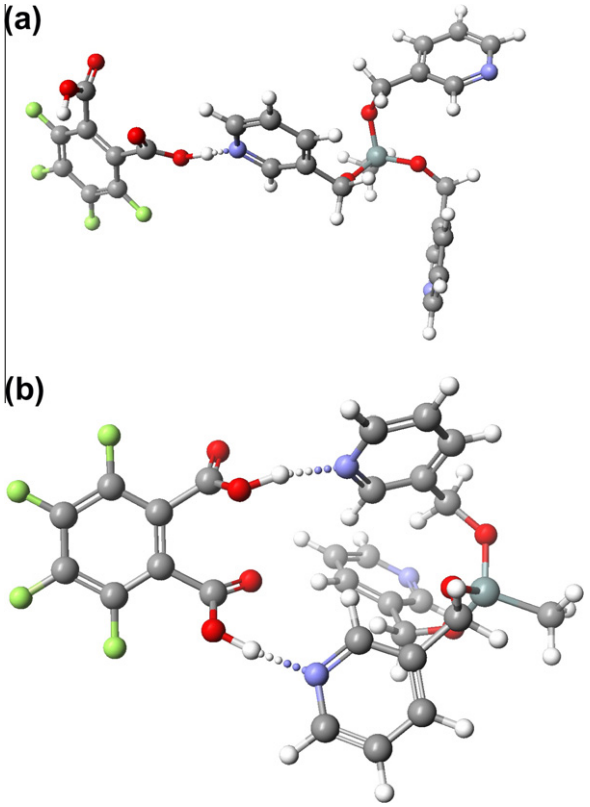


Fig. 3. Calculated (PM5) structure of DKFBo with ligand (8): (a) with one hydrogen bond and (b) with two hydrogen bonds.

systems with acids tetrafluorophtalic acids. The magnitude of these changes does not depend on receptor structure, but only slightly depends on the structure of tetrafluorophtalic acids. This result is surprising because it shows that the structures of dicarboxylic acids and Si-podands pyridylmethyl do not play significant role in the formation of complexes with hydrogen bonding. All the

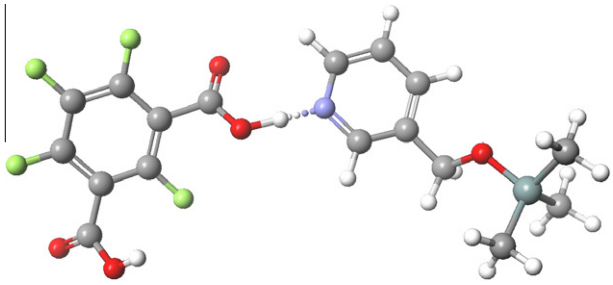


Fig. 4. Calculated (PM5) structure of DKFBm with ligand (2) with one hydrogen bond.

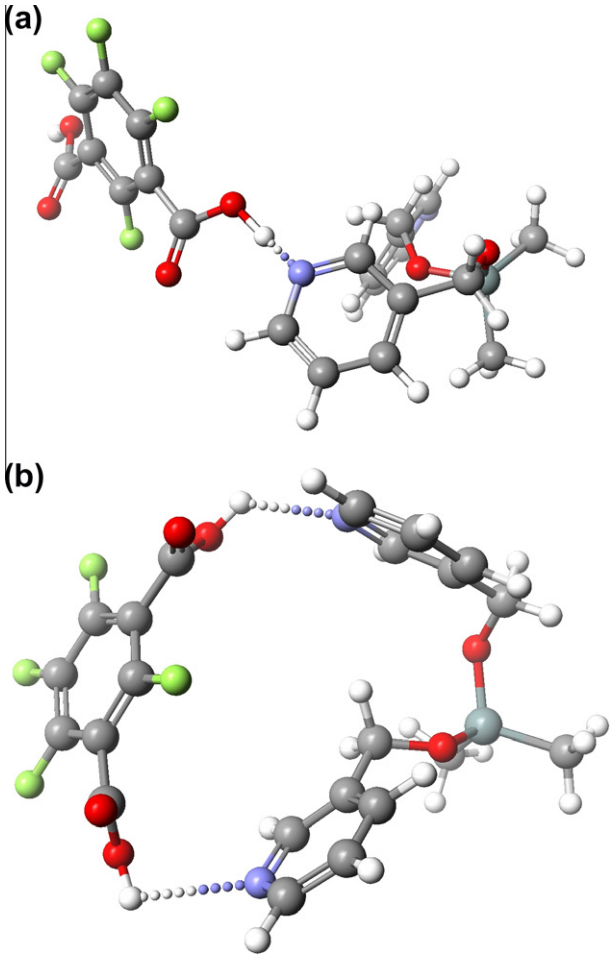


Fig. 5. Calculated (PM5) structure of DKFBm with ligand (5): (a) with one hydrogen bond and (b) with two hydrogen bonds.

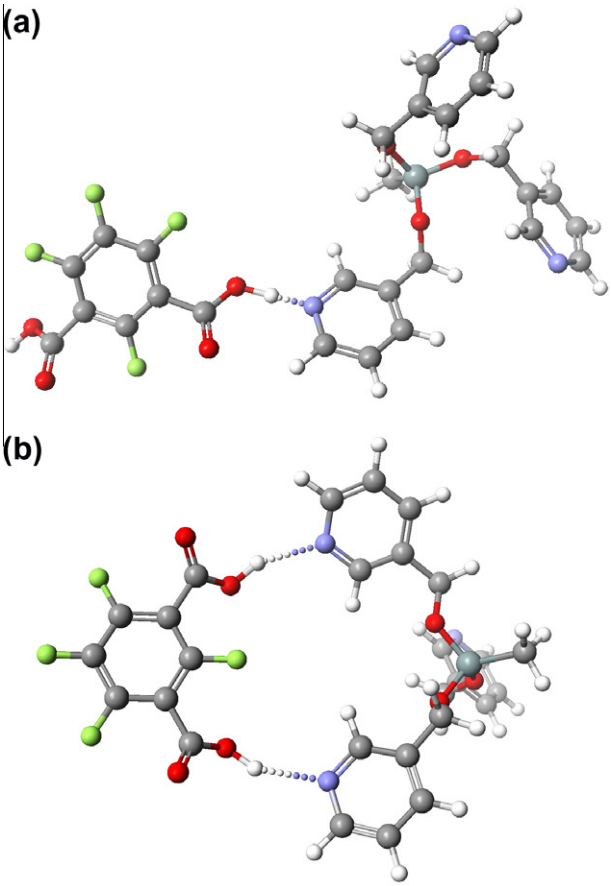


Fig. 6. Calculated (PM5) structure of DKFBm with ligand (8): (a) with one hydrogen bond and (b) with two hydrogen bonds.

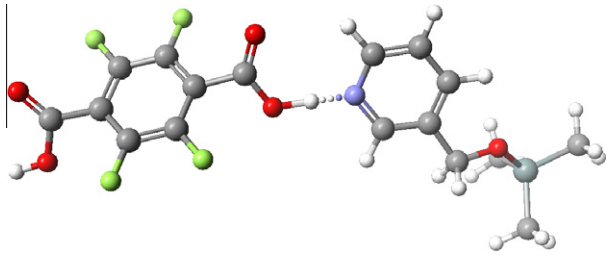


Fig. 7. Calculated (PM5) structure of DKFBp with ligand (2) with one hydrogen bond.

systems tested make hydrogen bonding complexes of similar structures.

In the system studied three types of complexes can be formed (Fig. 1A–C).

The structures of these complexes is shown in Fig. 1.

In the 1:1 complex of the acid and pyridine there is one hydrogen bond made between one carboxyl group of dicarboxylic acid and ligand involving the free electron pair of the nitrogen atom from pyridine ring (Fig. 1A). In the 1:1 complex of the second type, two carboxyl groups from dicarboxylic acid make two hydrogen bonds with two nitrogen atoms from pyridine rings in one ligand molecule (Fig. 1B). In the third type (Fig. 1C) 1:2 complex of acid: pyridimethyl Si podand, the complex is formed between two ligands and one acid molecule. Pyridylmethyl Si-podands belong to ligands with labile base group from pyridine, which easily fits the structure of dicarboxylic acid, irrespective of the position of nitrogen atom in the pyridine ring. In order to establish the types of complexes formed in the systems studied, for selected systems the hydrogen bond energies and lengths were calculated PM5 method. (Table 7 and Figs. 1–9).

For all systems selected for the calculations, the most energetically favorable complex is that of 1:2 stoichiometry of acid: pirydylmethyl Si-podands. Formation of intermolecular structures is much preferred over that of intramolecular ones (see Table 8).

The structure of the ligand with a labile basic center and that of dicarboxylic acid have insignificant role in formation of hydrogen bond complexes.

For m- and p-systems, chelates can be formed but their formation creates much tension is less energetically favorable than those with single hydrogen bonds.

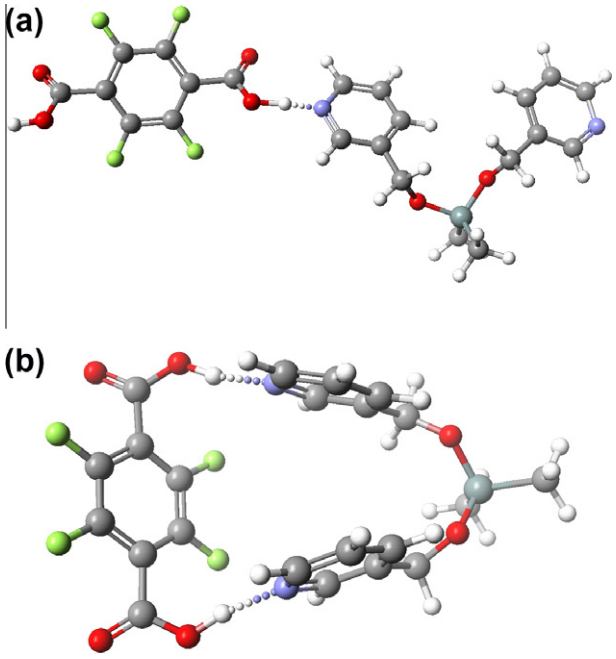


Fig. 8. Calculated (PM5) structure of DKFBp with ligand (5): (a) with one hydrogen bond and (b) with two hydrogen bonds.

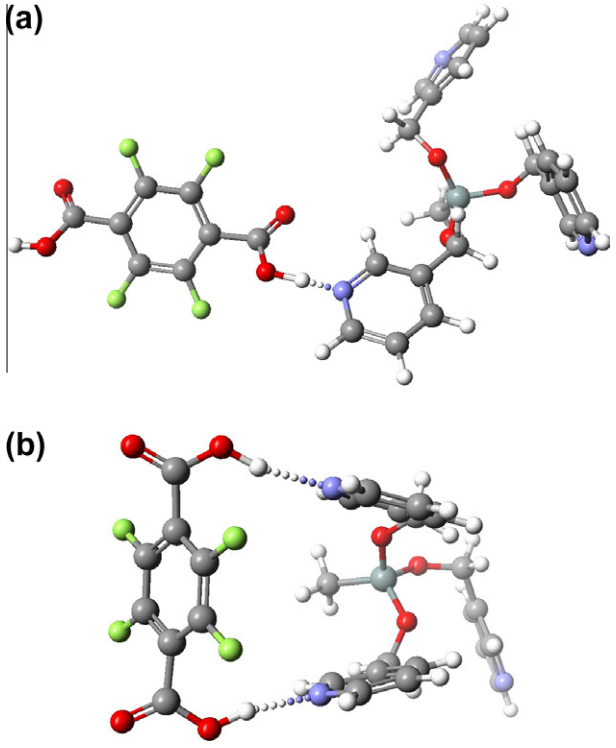


Fig. 9. Calculated (PM5) structure of DKFBp with ligand (8): (a) with one hydrogen bond and (b) with two hydrogen bonds.

As follows from the data displayed in Table 7, the most energetically favorable are the hydrogen bonds in the o-, and then in p- and m-systems. It is a consequence of the charge distribution in the acid ring and the resonance effects which affect the electron densities on the carboxyl groups. For the complexes characterized in Table 7, the acidity of protons increases in the series m < p < o, which influences which influences the strength of hydrogen bonds formed.

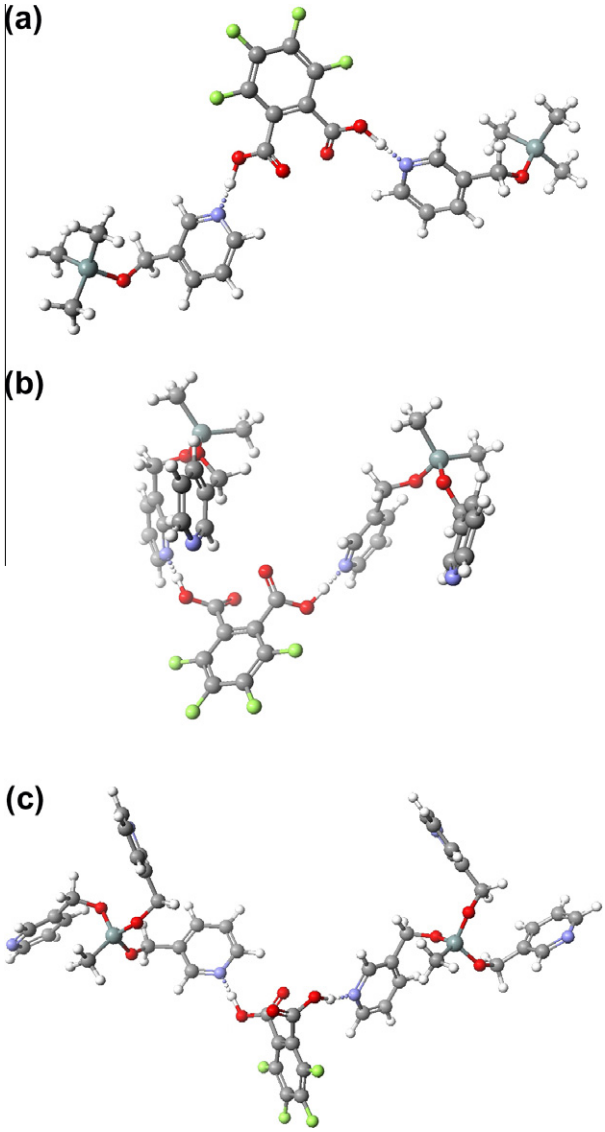


Fig. 10. Calculated (PM5) structure of DKFBo with two ligands: (a) 2, (b) 5, (c) 8.

Table 8
The theoretical parameters interaction between silane ligands and tetrafluorophtalic acid (**DKFBo**) in 2:1 stoichiometry.

Symbol of adduct	ΔHOF (kJ/mol)*
DKFBo + 2	−88.59
DKFBo + 5	−92.37
DKFBo + 8	−95.47

$\Delta HOF = HOF_{B\cdots HAH\cdots B} - HOF_{AH2+2B}$.

Acknowledgment

Authors thank the Polish Ministry of Science and Higher Education for financial support under Grant No. NN 204 338237 in the years 2009–2013.

References

[1] E. Epifani, S. Florio, L. Troisi, Tetrahedron 46 (1990) 4031.
[2] K. Tamao, N. Ishida, M. Kumada, J. Org. Chem. 48 (1983) 2120.
[3] F. Shirini, M.A. Zolfigol, M. Paktinat, Synthesis 24 (2006) 4252.
[4] M. Moghadam, S. Tangestaninejad, V. Mirkhani, I. Mohammadpoor-Baltork, S. Chahardahcheric, Z. Tavakoli, J. Organomet. Chem. 693 (2008) 2041.

[5] G. Schroeder, B. Gierczyk, B. Łęska, J. Incl. Phenom. 35 (1999) 327.
[6] A. Maia, D. Landini, B. Łęska, G. Schroeder, Tetrahedron 60 (2004) 10111.
[7] B. Łęska, R. Pankiewicz, B. Gierczyk, G. Schroeder, B. Brzezinski, J. Mater. Sci. 43 (2008) 3459.
[8] B. Łęska, R. Pankiewicz, G. Schroeder, A. Maia, J. Mol. Catal. A: Chem. 269 (2007) 141.
[9] B. Łęska, R. Pankiewicz, B. Gierczyk, G. Schroeder, J. Mol. Catal. A: Chem. 287 (2008) 165.
[10] J.L. Atwood, J.W. Steed (Eds.), Encyclopedia of Supramolecular Chemistry, Marcel Dekker, New York, 2004.
[11] G.W. Gokel, O. Murillo, in: J.L. Atwood, J.E.D. Davies, D.D. MacNicol, F. Vögtle (Eds.), Comprehensive Molecular Chemistry, vol. 1, Elsevier Science, Oxford, 1996.
[12] J.L. Sessler, P.A. Gale, W. Cho (Eds.), Anion Receptor Chemistry, RSCPublishing, Cambridge, 2006.
[13] P.D. Beer, D.P. Cormode, J.J. Davis, Chem. Commun. (2004) 414.
[14] M.H. Filby, J.W. Steed, Coord. Chem. Rev. 250 (2006) 3200.
[15] J.Y. Lee, M.H. Lee, K.S. Jeong, Supramol. Chem. 19 (2007) 257.
[16] C.M.G. Dos Santos, M. Glynn, T. McCabe, J.S. Seixas de Melo, H.D. Burrows, T. Gunnlaugsson, Supramol. Chem. 20 (2008) 407.
[17] A.P. Davis, Coord. Chem. Rev. 250 (2006) 2939.
[18] U.-I. Kim, J.-M. Suk, V.R. Naidu, K.-S. Jeong, Chem. - A Eur. J. 14 (2008) 11406.
[19] G.W. Lee, N. Singh, H.J. Jung, D.O. Jang, Tetrahedron Lett. 50 (2009) 807.
[20] V. Amendola, L. Fabbrizzi, Chem. Commun. 5 (2009) 513.
[21] C. Caltagirone, P.A. Gale, Chem. Soc. Rev. 38 (2009) 520.
[22] J.W. Steed, Chem. Soc. Rev. 38 (2009) 506.
[23] P.D. Beer, P.A. Gale, Angew. Chem. Int. Ed. 40 (2001) 486.
[24] R. Ludwig, N.T.K. Dzung, Sensors 2 (2002) 397.
[25] B. Kuswandi, Nuriman, W. Verboom, D.N. Reinhoudt, Sensors 6 (2006) 978.
[26] M.J. Berocal, A. Cruz, I.H.A. Badr, L.G. Bachas, Anal. Chem. 72 (2000) 5295.
[27] M.M. Meijler, R. Arad-Yellin, Z.I. Cabantchik, A. Shanzer, J. Am. Chem. Soc. 124 (2002) 12666.
[28] J. Kira, B. Łęska, G. Schroeder, P. Przybylski, B. Brzezinski, J. Mol. Struct. 738 (2005) 227.
[29] G. Schroeder, J. Kira, T. Ossowski, B. Łęska, P. Przybylski, B. Brzezinski, J. Mol. Struct. 788 (2006) 184.
[30] K. Choi, A.D. Hamilton, Coord. Chem. Rev. 240 (2002) 101.
[31] P.A. Gale, Coord. Chem. Rev. 213 (2001) 79.
[32] Ch.R. Bondy, S.J. Loeb, Coord. Chem. Rev. 240 (2003) 77.
[33] A.J. Evans, S.E. Matthews, A.R. Cowley, P.D. Beer, Dalton Trans. 24 (2003) 4644.
[34] T. Zieliński, P. Dydio, J. Jurczak, Tetrahedron 64 (2008) 568.
[35] M.G. Chudzinski, C.A. McClary, M.S. Taylor, J. Am. Chem. Soc. 133 (2011) 10559.
[36] M. Wenzel, M.E. Light, A.P. Davis, P.A. Gale, Chem. Commun. 47 (2011) 7641.
[37] T. Yamada, H. Kitagawa, Supramol. Chem. 23 (2011) 315.
[38] Y. Haketa, S. Sakamoto, K. Chigusa, T. Nakanishi, H. Maeda, J. Org. Chem. 76 (2011) 5177.
[39] Q. Li, Y. Guo, J.S. Shao, Sens. Actuat. B: Chem. 158 (2011) 427.
[40] A.S. Singh, B.-Y. Chen, Y.-S. Wen, C. Tsai, S.-S. Sun, Org. Lett. 11 (2009) 1867.
[41] S. Bao, W. Gong, W. Chen, J. Ye, Y. Lin, G. Ning, J. Incl. Phenom. Macrocycl. Chem. 70 (2011) 115.
[42] S.K. Dey, A. Pramanik, G. Das, Cryst. Eng. Comm. 13 (2011) 1664.
[43] M. Arunachalam, P. Ghosh, Chem. Commun. (2009) 5389.
[44] K. Salorinne, D.P. Weimann, C.A. Schalley, M. Nissinen, Eur. J. Org. Chem. (2009) 6151.
[45] S. Metzger, B. Lippert, J. Am. Chem. Soc. 118 (1996) 12467.
[46] T. Steiner, W. Saenger, J. Am. Chem. Soc. 114 (1992) 10146.
[47] C.V.K. Sharma, G.R. Desiraju, J. Chem. Soc. Perkin Trans. 2 (1994) 2345.
[48] G.J. Durant, J.C. Emmett, C.R. Ganellin, P.D. Miles, M.E. Parsons, H.D. Prain, G.R. White, J. Med. Chem. 20 (1977) 901.
[49] C.G. McCarty, R.V. Chastain, D.M. Wieland, J. Chem. Soc. D (1971) 198.
[50] S. Boverie, M.-H. Antoine, F. Somers, B. Becker, S. Sebille, R. Ouedraogo, S. Counerotte, B. Pirotte, P. Lebrun, P. de Tullio, J. Med. Chem. 48 (2005) 3492.
[51] MO-G Version 1.1, Fujitsu Limited, Tokyo, Japan, 2008.