Schiff base functionalized Organopropylsilatranes: Synthesis and structural characterization

GURJASPREET SINGHa,*, PROMILAA, AMANDEEP SAROA, JANDEEPSINGHA, RAJPalSHARMAB and V FERRETTIB

aDepartment of Chemistry and Centre of Advanced Studies in Chemistry, Panjab University, Chandigarh 160 014, India
bCenter for Structural Diffractometry and Department of Chemical and Pharmaceutical Sciences, University of Ferrara, via Fossato di Mortara 17-27, I-44100 Ferrara, Italy
e-mail: gjsingh@pu.ac.in

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Abstract. Synthesis of Schiff bases linked to organopropylsilatranes were performed by condensation reaction of post-functionalized silatranes such as aminopropylsilatran (4), aminopropyl-3,7,10-trimethylsilatran (5) and N-substituted aminopropylsilatran (10) with two different aldehydes viz. pyrole-2-carboxaldehyde and 2-hydroxy-1-naphthaldehyde. The resulting Schiff base substituted silatranes were well characterized by elemental analysis, spectroscopic studies [IR, (1H, 13C) NMR, and MS]. The structures of two silatranes were confirmed by single crystal X-ray diffraction analysis.

Keywords. Schiff base; 3-aminopropylsilatran; 3-aminopropyltriethoxysilane; pyrrole-2-carboxaldehyde; 2-hydroxy-1-naphthaldehyde.

1. Introduction

Silatranes are cyclic organosilicon ethers of trialkoxyamines which form a unique class of penta-coordinate silicon compounds. The focus of the interest in silatranes arises due to stereo-electronic influence of exocyclic fragment on the shape and reactivity pattern.

Since, introduction in 1961 by Frye et al.,1 studies on silatranes have been diversified owing to their potential applications in the field of medicine, agriculture, polymer science and material chemistry.2–5 The modification in exocyclic arm of silatranes advance the fundamental properties of a silatranes, such as their response towards hydrolysis, crystal packing and uses in biology and medicine.6–15 Only a few silatranes with Schiff base moiety substituted at axial positions have been reported.16–18

Schiff bases form an important class of synthetic organic compounds and are characterized by the presence of azomethine group. Moreover, they form important intermediates in some of the enzymatic reactions.19 Schiff bases are extensively studied due to pharmacological activity as anti-bacterial, anti-tumor, anti-inflammatory, anti-fungal, anti-HIV, analytical metal ion sensors and as catalysts.20–24 Moreover, they have chelating tendency (bi or tridentate) and form complexes with various transition metals. Owing to their rapidity in synthesis and diversified applications, we herein report the synthesis of Schiff base functionalized silatranes. The resulting organosilatranes can find use as advanced and modified activity centers.

In this manuscript, synthesis of six Schiff base functionalized organopropylsilatranes (6–9) and (12–13) which were derived from the reaction of aminopropylsilatran (4), aminopropyl-3, 7, 10-trimethylsilatran (5) and N-substituted aminopropylsilatran (10) with two aldehydes viz. pyrrole-2-carboxaldehyde and 2-hydroxy-1-naphthaldehyde have been carried out. The molecular structures of silatran (6) and (12) were obtained by single crystal X-ray diffraction studies.

2. Experimental

2.1 Materials and methods

2.1a General details: Syntheses of all the compounds were performed under dry nitrogen atmosphere using Schlenk technique. All organic solvents were dried and purified according to standard procedures.

3-aminopropyltriethoxysilane (Aldrich), N-[3-(trimethoxysilyl)propyl]ethylendiamine (Aldrich), triethanolamine

*For correspondence
(Merck), pyrrole-2-carboxaldehyde (Aldrich), 2-hydroxynaphthaldehyde (Aldrich) and trisopropanolamine (Merck) were distilled prior to use. 3-aminopropylsilatrane (4), aminopropyl-3, 7, 10-trimethylsilatrane (5) and N-substituted aminopropylsilatrane (10) were synthesized by the methods reported in literature.

The infrared spectra were recorded using Nicolet iS50 FTIR (Fourier Transform Infra-Red) spectrometer. Mass spectral measurements (ESI source with capillary voltage, 2500 V) were carried out on a VG Analytical (70-S) spectrometer. CHN analyses were obtained on a FLASH-2000 Organic Elemental Analyzer. The solution NMR spectra were recorded on Bruker Avance II FT NMR (AL 300 MHz) spectrometers (1H, 13C) using CDCl3 as the solvent. Chemical shifts in ppm were reported relative to tetramethylsilane (TMS).

2.1b X-ray crystallography: Single crystal diffraction data for compounds 6 and 12 were collected on a Nonius Kappa CCD diffractometer equipped with a CCD detector with graphite-monochromatized MoKa radiation (λ = 0.71073 Å). All intensities were corrected for Lorentz and polarization effects. The structures were solved by direct methods with the SIR97 program and refined on F2 by full-matrix least-squares methods with anisotropic non-H atoms.

In 6, the N3-H hydrogen atom was located in the difference-fourier map and its coordinates were kept fixed during the refinement. In 12, the hydrogen atoms linked to N2, N4 and C17 were located in the difference-fourier map and refined isotropically. All other hydrogens of both structures were included on calculated positions, riding on their carrier atoms. In structure of compound 12, atoms C1, C3 and C5 were found to be disordered over two almost equivalent positions (60-40%). All other calculations were accomplished using SHELX97 and WINGX. Crystal data and refinement details are given in Table 1.

2.2 Synthesis of silatranes

2.2a N-{((1H-pyrrol-2-yl)methylene)-3-(2,8,9-trioxa-aza-1-sila-bicyclo[3.3.3]undecan-1-yl)propan-1-amine (6): 3-aminopropylsilatrane (1.00 g, 4.31 mmol) was dissolved in toluene and pyrrole-2-carboxaldehyde (0.41 g, 4.31 mmol) was added to the uniformly stirred pre-dissolved reaction mixture. The mixture was refluxed for 2 h and water formed during the reaction was removed azeotropically from the reaction solution by Dean-Stark assembly. Toluene was evaporated and off-white colored solid appeared which was dried under reduced pressure. Crystals suitable for X-ray diffraction were obtained from chloroform/benzene. Yield: 82%, 1.09 g, M.p.: 156 – 158°C. Anal. Calcd (%) for C16H23N3O4Si: C, 54.36; H, 7.44; N, 13.59, Si, 9.06; Found(%): C, 54.37, H, 7.45; N, 13.53; Si, 9.08; IR (KBr pellet, cm⁻¹): ν = 579.7 (Si–N), 751.5 (Si-O), 879.3 (C=N), 937.9 (C-C), 1088.3 (Si-O), 1130.3 (C-O), 1633.9 (C-N), 2873.9 s, 2937.6 (CH2). 1H NMR (300 MHz, CDCl3): δ = 0.34 (2H, m, SiCH2), 1.66 (2H, m, CCH2), 2.71 (6H, t, JHH 5.4Hz NCH2), 3.44 (2H, m, CCH2N), 3.67 (6H, t, JHH 5.1 Hz, OCH2), 7.97 (s, 1H, N=CH), 6.09-6.78 (3H, m, Ar-H). 13C NMR (75 MHz, CDCl3): δ = 13.2 (SiCH3), 26.5 (CCH2), 51.5 (CCH2N), 58.0 (NCH2), 64.1 (OCH2), 75.7 (CCH2), CDCl3: δ = 13.2 (SiCH3), 26.5 (CCH2), 51.5 (CCH2N), 58.0 (NCH2), 64.1 (OCH2), 121.17 (C2, C3-pyrrole), 128.3 (C1, C4-pyrrole), 151.0 (N=CH). MS (309): m/z: 310[M+H]+, 311[M+2H]+.

Table 1. Experimental details.

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<tr>
<td>Z</td>
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<td>4</td>
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<tr>
<td>μ (mm⁻¹)</td>
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<td>0.47</td>
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<td>0.050</td>
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<td>0.069, 0.238, 1.02</td>
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<td>5480</td>
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<td>No. of parameters</td>
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<td>292</td>
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<td>Δρ_max, Δρ_min (e Å⁻³)</td>
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<td>0.48 – 0.54</td>
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2.2b N-((1H-pyrrol-2-yl)methylene)-3-(3,7,10-trimethyl-2,8,9-trioxo-5-aza-1-sila-bicyclo[3.3.3]undecan-1-yl)propan-1-amine (7): 3-aminopropyl-3,7,10-trimethylsilatranate (1.00 g, 3.65 mmol) was dissolved in toluene and pyrrole-2-carboxaldehyde (0.35 g, 3.65 mmol) was added to pre-dissolved stirred reaction mixture. The mixture was refluxed for 2 h and water formed during the reaction was removed azeotropically from the reaction solution by Dean Stark assembly. Toluene was evaporated and light brown coloured solid appeared which was dried under reduced pressure. Yield: 76%, 0.97 g, M.p.: 160-162°C. Anal. Calc. (%): C, 58.29; H, 8.00; N, 12.00; Si, 8.00; Found (%): C, 58.25; H, 8.01; N, 12.01; Si, 8.02; IR (KBr pellet, cm⁻¹): 579.2 ν (Si–N), 750.9 ν (Si–O), 877.6 ν (C–N), 937.2 ν (C–C), 1086.9 ν (Si–O), ν (Si–O), 1178.9 (C–O), 1605.3 ν (C–N), 2873.2 s, 2934.5 (v, CH₂); ¹H NMR (300 MHz, CDCl₃): δ = 0.33 (2H, m, Si–CH₂), 1.13 (2H, m, C–CH₂), 2.73 (6H, t, JHH 5.4 Hz, NCH₂), 2.91 (2H, m, C–CH₂), 0.92 (9H, dt, CH₃), 2.73 (3H, m, OCH), 7.30 (1H, s, N=CH), 5.52-6.82 (3H, m, Ar-H). ¹³C NMR (75 MHz, CDCl₃): δ = 14.0 (SiCH₃), 52.0 (CH₃), 151.1 (C₄-alkyl), 151.8 (N=CH). MS (350): m/z; 351 [M+H]+, 352 [M+2H]+.

2.2c 2-((3-(2,8,9-trioxo-5-aza-1-sila-bicyclo[3.3.3]undecan-1-yl)propylin) methyl)naphthalen-1-ol (8): 3-aminopropylsilatranate (1.00 g, 4.31 mmol) was dissolved in toluene and 2-hydroxy-1-naphthaldehyde (0.62 g, 4.31 mmol) was added pre-dissolved stirred reaction mixture. The mixture was refluxed for 2 h and water formed during the reaction was removed azeotropically from the reaction solution by Dean Stark assembly. Toluene was evaporated and light yellow colored solid appeared which was dried under reduced pressure. Yield: 64%, 1.10 g, M.p.: 164-166°C. Anal. Calc. (%): C, 60.15; H, 6.26; N, 10.52; Si, 7.01; Found (%): C, 60.11; H, 6.28; N, 10.50; Si, 7.00; IR (KBr pellet, cm⁻¹): ν = 567.4 (Si–N), 741.2 (Si–O), 864.7 (C–N), 1010.6 (C–C), 1074.5 (Si–O), 1258.7 (C–O), 1591.5 (C=N), 2888.5 s, 2962.0 (CH₃). ¹H NMR (300 MHz, CDCl₃): δ = 0.38 (2H, m, Si–CH₂), 1.72 (2H, m, C–CH₂), 2.68 (6H, t, JHH 5.4 Hz, NCH₂), 3.49 (2H, m, C–CH₂), 3.66 (6H, t, JHH 5.4 Hz, OCH₂), 8.55 (1H, s, N=CH), 6.73-7.01 (m, Ar-H). ¹³C NMR (75 MHz, CDCl₃): δ = 12.9 (Si–CH₂), 26.8 (C–CH₂), 51.3 (C–CH₂), 55.4 (N–CH₂), 57.7 (O–CH₂), 157.0 (C₁-naphthol), 100.7 (C₂-naphthol), 136.9 (C₃-naphthol), 126.0 (C₄, C₅-naphthol), 122.0 (C₆-naphthol), 127.6 (C₇-naphthol), 129.1 (C₈, C₉-naphthol), 117.6 (C₁₀-naphthol), 163.8 (N=CH). MS (399): m/z; 422[M+Na]+.

2.2d 2-((3-(3,7,10-trimethyl-2,8,9-trioxo-5-aza-1-sila-bicyclo[3.3.3]undecan-1-yl)propylin) methyl)naphthalen-1-ol (9): 3,7,10 trimethyl substituted amino-propylsilatranate (1.00 g, 4.31 mmol) was dissolved in dry toluene and 2-hydroxy napthaldehyde (0.44 g, 4.31 mmol) was added to pre-dissolved stirred reaction mixture. The mixture was refluxed for 2 h and water formed during the reaction was removed azeotropically from the reaction mixture by Dean Stark apparatus. Toluene was evaporated and yellowish colored solid appeared which was dried under reduced pressure. Yield: 62%, 0.97 g, M.p.: 168-169°C. Anal. Calc. (%): C, 64.48; H, 7.47; N, 6.54; Si, 6.54; Found (%): C, 64.49; H, 7.45; N, 6.55; Si, 6.53; IR (KBr pellet, cm⁻¹): ν = 687.2 (Si–N), 1094.7 (Si–O), 1191.9 (C–O), 1631.7 (C=N), 2868.1, 2924.6 (CH₂). ¹H NMR (300 MHz, CDCl₃): δ = 0.63 (2H, m, Si–CH₂), 1.28 (2H, m, C–CH₂), 2.76 (6H, t, JHH 5.4 Hz, NCH₂), 3.00 (2H, m, C–CH₂), 0.96 (9H, dt, CH₃), 2.05 (3H, m, OCH), 8.30 (1H, s, N=CH), 6.21-7.40 (m, Ar-C). ¹³C NMR (75 MHz, CDCl₃): δ = 14.5 (Si–CH₃), 25.5 (CH₃), 38.1 (C–CH₂), 40.1 (C–CH₂), 50.0 (NCH₂), 60.4 (OCH), 152.0 (C₁-naphthol), 100.7 (C₂-naphthol), 129.9 (C₃-naphthol), 128.1 (C₄, C₅-naphthol), 121.6 (C₆-naphthol), 128.1 (C₇-naphthol), 129.9 (C₈, C₉-naphthol), 110.3 (C₁₀-naphthol), 163.4 (N=CH). MS (428): m/z; 429[M+H]+, 430[M+2H]+.

2.2e N⁰-((1H-pyrrol-2-yl)methylene)-N⁰-((3-(2,8,9-trioxo-5-aza-1-sila-bicyclo[3.3.3]undecan-1-yl)propylin) ethane-1,2-diamine (12): N⁰-((3-(2,8,9-trioxo-5-aza-1-sila-bicyclo[3.3.3]undecan-1-yl)propylin)ethane-1,2-diamine (1.00 g, 3.63 mmol) was dissolved in dry toluene and pyrrole-2-carboxaldehyde (0.35 g, 3.63 mmol) was added to pre-dissolved reaction mixture. The mixture was refluxed for 2 h and water formed during the reaction was removed azeotropically from the reaction solution by Dean Stark assembly. Toluene was evaporated and light yellow colored solid appeared which was dried under reduced pressure. Crystals suitable for X-ray diffraction were obtained from chloroform/benzene. Yield: 86%, 1.10 g, M.p.: 167-168°C. Anal. Calc. (%): C, 54.54; H, 7.95; N, 15.90; Si, 7.95; Found (%): C, 54.52; H, 7.91; N, 15.92; Si, 7.99; IR (KBr pellet, cm⁻¹): 582.3 ν (Si–N), 752.8 ν (Si–O), 877.8 ν (C–N), 941.2 ν (C–C), 1097.3 ν (Si–O), ν 1182.3 (C–O), 1636.0 ν (C=N), 2871.9 s, 2926.7 (v, CH₃). ¹H NMR (300 MHz, CDCl₃): δ = 0.39 (2H, m, Si–CH₂), 1.59 (2H, m, C–CH₂), 2.63 (2H, m, C–CH₂), 2.77 (6H, t, JHH 5.4 Hz, NCH₂), 3.61 (2H, m, C–CH₂), 3.74 (6H, t, JHH 5.4 Hz, OCH₂), 8.07 (1H, s, N=CH), 6.21-7.36 (3H, m, Ar-H). ¹³C NMR (100.62 MHz, CDCl₃): δ = 13.4 (Si–CH₂), 25.1 (C–CH₂), 49.8 (C–CH₂).
2,2′-((2-(3-(2,8,9-trioxo-5-aza-1-sila-bicycle[3.3.3] undecan-1-yl)propylamino)ethylamino)methyl)naphthalen-1-ol (13): N1-(3-(3,7,10-trimethyl-2,8,9-trioxo-5-aza-1-sila-bicycle[3.3.3]undecan-1-yl)propyl)ethane-1,2-diamine (1.00 g, 3.63 mmol) was dissolved in toluene and 2-hydroxynaphthaldehyde (0.62 g, 3.63 mmol) was added to pre-dissolved reaction mixture. The mixture was refluxed for 2 h and water formed during reaction was removed azeotropically from the reaction solution by Dean Stark assembly. Toluene was evaporated and reddish yellow colored solid appeared which was dried under reduced pressure. Yield: 58%, 0.90 g. M.p.: 170-172°C; Anal. Calcd(%): for C22H31N2O2Si: C, 61.53; H, 7.22; N, 9.79; Si, 6.52; Found(%): C, 61.52; H, 7.25; N, 9.80; Si, 6.54; IR (KBr pellet, cm⁻¹): 582.3 ν (Si←N), 749.6 ν (Si-O), 585.4 ν (C-N), 937.8 ν (C-C), 1083.6 ν (Si-O), 1178.0 (C-O), 1625.1 ν (C=N), 2872.1 s, 2924.1 (υ, CH2), 3H NMR (300 MHz, CDCl₃): δ = 0.33 (2H, m, SiCH₂), 1.26 (2H, m, CCH₃C), 1.72 (2H, m, NCH₂CH₂), 2.80 (6H, t, J₉₈ 5.4 Hz, NCH₂), 3.61 (2H, m, CCH₂N), 3.75 (6H, t, J₉₈ 5.4 Hz, OCH₂), 8.11 (1H, s, N=CH), 6.13-7.69 (m, Ar-H). 13C NMR (75 MHz, CDCl₃): δ = 133.4 (SiCH₂), 26.2 (CCH₂C), 46.4 (CCH₂N), 51.0 (NCH₂CH₂), 57.6 (NCH₂), 76.7 (OCH₂), 163.3 (C1-naphthol), 94.5 (C2-naphthol), 129.0 (C3-naphthol), 128.3 (C4, C5-naphthol), 121.6 (C6-naphthol), 129.7 (C7-naphthol), 129.7 (C8, C9-naphthol), 110.1 (C10-naphthol), 163.3 (N=CH). MS (429): m/z; 430[M+H]⁺.

3. Results and Discussion

3.1 Synthetic aspects

The strategic approach towards the synthesis of Schiff bases bearing organosilicon moiety with different structures was based on condensation reaction between 3-aminopropylsilatrane and different aromatic aldehydes. Synthesis of Schiff bases substituted organosilicon complexes have been carried out by the reaction of aminopropylsilatrane (4), aminopropyl-3,7,10-trimethylsilatrane (5) and N-substituted aminopropylsilatrane (10) with various aldehydes viz. pyrrole-2-carboxaldehyde, 2-hydroxy naphthaldehyde (scheme 1). These new ‘Schiff modified silatrane’ have been characterized by elemental analysis IR, (1H, 13C) NMR spectroscopy and mass spectrometry.

Synthesis of Schiff base bearing silatrane (12, 13) were also carried out by using N-substituted aminopropylsilatrane (11) with increased number of carbon atoms with aromatic aldehydes like pyrrole-2-carboxaldehyde, 2-hydroxy naphthaldehyde as shown in scheme 2. The structure of silatrane (6) and (12) has been deduced by single crystal X-ray diffraction analysis.

Scheme 1. Synthesis of Schiff bases linked silatrane from 3-aminopropylsilatrane.
3.2 Spectroscopic Studies

3.2a FT-IR spectroscopy: The formation of the silatranes 6–9, 12 and 13 was established by FTIR spectroscopy. The most characteristic absorption bands associated with silatran structure were found in the spectrum of all the silatranes. IR spectra of all compounds (6–9, 12, 13) exhibit absorption bands characteristic to both C=N of Schiff base and silatranyl moiety. Bands observed in the region of 3200-3400 cm\(^{-1}\) are assigned to OH stretching modes, whereas C=N stretching vibrations are observed at 1591-1636 cm\(^{-1}\). The intense bands were present in the region 1086-1094 cm\(^{-1}\) and are assigned to asymmetric stretching vibration of the Si-O group. In addition, a Si←N vibration observed in the region 567-687 cm\(^{-1}\) is a common feature of silatranes.

3.2b NMR spectroscopy: The multinuclear NMR spectra of all compounds were consistent with the structure of the synthesized complexes (6–9, 12, 13). The NMR spectra of silatranyl moiety of the synthesized compounds (6, 8, 12, 13) were very similar to their parent compounds and consisted of triplets due to protons of OCH\(_2\) \(\delta\) (3.66–3.74 ppm) and NCH\(_2\) \(\delta\) (2.68–2.80 ppm) of Si(OCH\(_2\)CH\(_2\))\(_3\)N moiety. The \(^1\)H NMR spectra of all the synthesized compounds (6–9, 12, 13) show singlet in the region \(\delta\) 7.46–8.55 due to -N=CH moiety of Schiff base bearing silatranes (6–9) and (12, 13) which signifies successful condensation reaction. The methyne proton (CH) of the isopropyl group appears at \(\delta\) 2.05–2.73 ppm since, it is adjacent to six equivalent hydrogens (the two isopropyl CH\(_3\) groups) and the signals for the two (magnetically equivalent) CH\(_3\) groups were ascribed at \(\delta\) 0.92–0.96 ppm by the adjacent methylene proton (CH). In \(^{13}\)C NMR, silatranes (6, 8, 12, 13), the resonances due to silatranyl OCH\(_2\) and NCH\(_2\) appears at \(\delta\) 64.14–76.71 ppm and \(\delta\) 56.52–58.06 ppm, respectively. In the 3,7,10-trimethylsilatranes (7, 9), the signals ascribed to NCH\(_2\) are at 50.03 and 56.22 ppm, respectively whereas OCH appears slightly downfield at \(\delta\) 50.03 and 56.22 ppm, respectively. The signals due to the carbon atoms attached to the azomethine groups in compounds (6–9) and (12, 13) appear in the range \(\delta\) 151.00–163.6 ppm, respectively.

3.2c Mass spectrometry: Mass spectra of compounds (6–9) and (12,13) show molecular ion peaks with addition of H\(^+\), Na\(^+\) and K\(^+\) ions and their fragmentation
exhibit common features of silatranes.⁵⁰ The silatranes reported herein possess considerable stability, as indicated by the continuous observation of a strong \([\text{M} + \text{H}]^+\) as a base peak.

3.3 Single crystal X-ray structure analysis

Figures 1 and 2 report the ORTEP III diagram for compounds 6 and 12, respectively. Relevant geometrical parameters are reported in table 2. In 6, the asymmetric unit is formed by a silatran molecule and a half of a benzene molecule, the C15 and C18 atoms of the solvent molecule being positioned on a two-fold rotation axis, while in 12, it is composed by a silatran moiety and one chloroform solvent molecule. In both structures the silicon atom is linked in distorted trigonal bipyramidal geometry (see table 2) to the tripodal triethanolamine ligand, with Si-O and Si-N distances typical for this kind of compounds. Actually, the Si-O and Si-N mean bond lengths calculated on 146 silatran structures present in CSD are 1.66(1) and 2.15(5) Å, respectively.

The main interactions in both structures are represented by N-H...N hydrogen bonds, which give origin to dimeric units (table 3). Very interestingly, the cocrystallized solvent molecules, benzene in 6 and chloroform

Figure 1. ORTEP III view and atom numbering scheme for compound 6. Thermal ellipsoids are drawn at the 40% probability level. C-H...π contact is drawn as dashed lines.

Figure 2. ORTEP III view and atom numbering scheme for compound 12. Thermal ellipsoids are drawn at the 40% probability level. For the sake of clarity, only one set of the disordered part has been considered.
in 12, are included in the crystalline lattice in such a way to act as linkers among the different dimers. In 6, C–H...π interactions are formed involving the C10-H atom of two symmetrically related silatrane molecules and the solvent, as shown in figure 3a, with the following geometrical parameters: H...C15-C18 (centroid) = 3.134 Å, C-H...centroid = 148°. Conversely, in 12, the chloroform acts both as a donor and as an acceptor group, being involved in a C17-H...O3 and in C10-H...Cl3 weak hydrogen bonds with two different silatrane molecules (table 3 and figure 3). This same chloroform silatrane interaction was found in the related compound CABBEN.\textsuperscript{32} Here, DFT calculations have shown the effective importance of the presence of the solvent molecule and the related interactions for the packing energy of the crystal.

**Table 2.** Selected bond distances and angles (Å, °).

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<td>Si1 - N1</td>
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<td>2.147(4)</td>
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<tr>
<td>O1 - Si1 - C7</td>
<td>97.3(2)</td>
<td>97.0(1)</td>
</tr>
<tr>
<td>O2 - Si1 - O3</td>
<td>117.8(2)</td>
<td>117.8(1)</td>
</tr>
<tr>
<td>O2 - Si1 - C7</td>
<td>96.8(2)</td>
<td>96.5(2)</td>
</tr>
<tr>
<td>O3 - Si1 - C7</td>
<td>99.5(2)</td>
<td>97.3(1)</td>
</tr>
<tr>
<td>O1 - Si1 - N1</td>
<td>81.9(1)</td>
<td>83.1(1)</td>
</tr>
<tr>
<td>O2 - Si1 - N1</td>
<td>82.3(2)</td>
<td>83.1(1)</td>
</tr>
<tr>
<td>O3 - Si1 - N1</td>
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<td>83.0(1)</td>
</tr>
<tr>
<td>N1 - Si1 - C7</td>
<td>178.3(2)</td>
<td>179.6(1)</td>
</tr>
</tbody>
</table>

**Figure 3.** Interactions involving the solvent molecules in 6 (a) and 12 (b).

4. Conclusions

A new class of silatrane (6-9) and (12, 13) bearing Schiff base moieties were synthesized and characterized by various spectroscopic techniques. These compounds containing azomethine group are bonded to the silicon’s axial position through propyl chain. The molecular structures of compounds (6) and (12) were obtained from single X-ray crystallography.

**Supplementary Information (SI)**

CCDC 1012013 and 1012014 contain the supplementary crystallographic data for complexes 6 and 12. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. Supplementary data associated with this article can be found, in the online version, at www.ias.ac.in/chemsci.
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