Vertical electron affinities in substituted trimethylsilanes

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Abstract

The gas-phase negative electron affinities obtained by means of electron transmission spectroscopy (ETS) in the series $(CH_3)_3Si-X$ (with X = I, Br, Cl, $Si(CH_3)_3$, SCH_3, OCH_3, $N(CH_3)_2$, CH_3) are compared. The electron-acceptor properties of these compounds increase when the substituent contains third-row (or heavier) elements. Geometries and charge distributions in the neutral molecules are calculated at the 3-21G* and 6-31G** ab initio levels (except for X = I, Br). The LUMO energies predicted by 3-21G*, 6-31G**, ΔSCF and semiempirical MNDO calculations are compared with the resonance energy trend observed in the ET spectra. © 1997 Elsevier Science S.A.

1. Introduction

Over the last decade, silicon-containing molecular systems have attracted great attention owing to their interesting mechanical and electronic properties. In particular, oligosilanes absorb in the UV region at sizeably lower energy with respect to the corresponding alkanes, their behaviour in this regard resembling more to that of unsaturated hydrocarbons. This reduced spectral band gap confers conducting properties to doped polysilanes. The peculiar and important properties of silicon catenates has stimulated many experimental and theoretical studies aimed at the characterisation of their electronic structure. Several ionisation energy measurements [1–4] by photoelectron spectroscopy provided a picture of the valence-filled orbitals in oligosilanes and permethylated derivatives, and demonstrated, in agreement with theoretical results, that the outermost filled MOs possess σ_{Si-Si} character and are strongly delocalised along the Si skeleton.

In contrast with the wealth of experimental information on the filled orbital structure, the corresponding data (vertical electron affinities, VEAs) on the empty orbitals are much rarer. In addition, theoretical evaluation of these data also presents difficulties [5]. We have recently reported [6] for the first time the energies of electron attachment (attachment energies, AEs, i.e., the

negative of the VEAs) to the low-energy empty orbitals in linear and branched permethylated oligosilanes, measured by means of electron transmission spectroscopy (ETS) [7]. In hexamethyldisilane, the presence of the Si–Si bond causes a sizeable electron affinity increase with respect to the corresponding hydrocarbon and to tetramethylsilane. The σ^*_{Si-Si} orbital (LUMO) is well separated in energy from the higher-lying σ^*_{Si-C} orbitals. The LUMO is progressively stabilised with increasing length of the Si chain and the energy splitting among the σ^*_{Si-Si} orbitals is even larger than that observed in their filled counterparts. These results fully account for the different spectral features of silanes and the relative stability of their radical anions with respect to saturated hydrocarbons.

Here, we extend the gas-phase ETS analysis to the $(CH_3)_3Si-X$ series to investigate the effects produced by various substituents on the electron-acceptor properties of the monosilane. The ET spectra of the compounds with X = halogen atom and $Si(CH_3)_3$ have been reported in our previous papers [8,6], while those of the SCH_3, OCH_3 and $N(CH_3)_3$ derivatives are presented for the first time. The discussion of the experimental data and the mechanisms of interaction between the silicon and substituent groups is aided by analysis of the geometries and charge distributions in the neutral states calculated at the ab initio 3-21G* and 6-31G** levels. The measured AEs are compared with the neutral state LUMO energies supplied by these methods and by

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semiempirical MNDO calculations, which satisfactorily reproduced the experimental energy trends in the above mentioned series of permethylated oligosilanes [6]. In addition, the neutral/anion energy differences at the neutral molecule geometry are evaluated with ΔSCF (6-31G * *) calculations. We do not employ calculations with diffuse functions, such as for instance 6-31 + G *, which demonstrated [9,10] to be inadequate for describing the resonance process, i.e., temporary electron attachment. The reason is that although these anion states are unstable with respect to electron detachment, during the resonance lifetime, the extra-electron is confined to the molecule by a centrifugal potential barrier. In contrast, the use of diffuse functions places the extra-electron as far as possible so that the predicted AE values are about the same for every molecular system.

Yoshimura and Tada [11] recently reported an ab initio study of the anion stabilities in a series of substituted silanes (H_3Si-X) similar to those considered here. If, on the one hand, apparent analogies exist between their paper and the present work, on the other hand, the different approaches used (theoretical and experimental, respectively) do not constitute the only substantial difference. Yoshimura and Tada calculated the adiabatic electron affinities, that is, the energy difference between neutral and anion states each in its minimum energy geometry. At variance, the physical process of electron capture, referred to as shape resonance, occurs through a vertical transition which leads to anion formation in the same geometry of the neutral state. Fig. 1 gives a schematic representation of the adiabatic and vertical electron affinity (AEA and VEA, respectively) and of the vertical ionisation potential (VIP) of the anion in its minimum geometry. The attachment energies measured in ETS are the negative of the vertical electron affinities, thus reflecting the ease of anion formation rather than their thermodynamic stability. These data are of great importance for an understanding of the electron-acceptor properties of neutral molecules or the reactivity of temporary anions (typical lifetime $10^{-10}-10^{-15}$ s) which often decay by giving up the extra electron or by dissociating before they can reach their equilibrium geometry.

2. Experiment and calculations

ETS is one of the most suitable means for measuring the negative vertical electron affinities of gas samples. This technique takes advantage of the sharp variations in the total electron-molecule scattering cross section caused by resonance processes, namely, temporary capture of electrons with appropriate energy and angular momentum. Our electron transmission apparatus is in the format devised by Sanche and Schulz [7] and has been previously described [12]. To enhance the visibil-
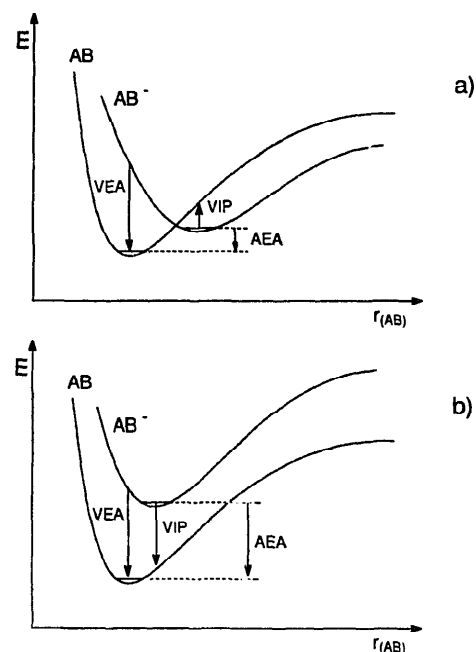

Fig. 1. Hypothetical potential curves for the ground neutral state of a molecule AB and its lowest anion state, in the case of large (a) and small (b) geometrical variations in the anion state. VEA = vertical electron affinity; AEA = adiabatic electron affinity; VIP = vertical ionisation potential of the anion in its minimum geometry. The downward and upward arrows are meant to represent the negative and positive signs, respectively, of the electron affinity and ionisation potential values.

ity of the sharp resonance structures, the impact energy of the electron beam is modulated with a small ac voltage, and the derivative of the electron current transmitted through the gas sample is measured directly by a synchronous lock-in amplifier. The spectra were obtained in the 'high-rejection' mode [13], and are, therefore, related to the nearly total scattering cross section. The electron beam resolution was about 50 meV (FWHM). The energy scales were calibrated with reference to the $(1s^12s^2)$ ^2S anion state of He. The estimated accuracy is ±0.05 or ±0.1 eV, depending on the number of decimal digits reported.

Molecular geometries and electron charge distributions for compounds $(CH_3)_3Si-X$, with $X = F$, Cl, $Si(CH_3)_3$, CH_3, $N(CH_3)_2$, OCH_3 and SCH_3, were computed at the ab initio 3-21G * and 6-31G * * levels. Relaxation of all the internal parameters at the 3-21G * level resulted in conformations without symmetry (C_1) but quite close to C_{3v} or C_s symmetry for the halogen and the $N(CH_3)_2$, OCH_3 and SCH_3 derivatives, respectively. When C_{3v} or C_s symmetry was forced, the total energy increased slightly, but the relevant geometrical parameters, the charge distributions and the electron energy levels did not change significantly. The data reported in the tables are those obtained allowing relaxation of all the internal parameters. The calculations for the $X = Si(CH_3)_3$ (D_{3d}) and CH_3 (T_d) derivatives were

already available [6]. At the 6-31G* * level, the geometry was optimised forcing C_{3v}, C_s, T_d or D_{3d} symmetry, as appropriate. The empty orbital energies, to be compared with experimental AE values within the Koopmans' theorem approximation, were computed by 3-21G*, 6-31G* * and MNDO calculations for the above compounds, including in the latter Br and I derivatives. Finally, the ΔSCF (6-31G* *) procedure was used to determine the energy difference between the ground state of each neutral molecule and that of its anion at the neutral molecule geometry.

3. Results and discussion

The ET spectra of the $(CH_3)_3Si-X$ compounds with $X = N(CH_3)_2$, OCH_3 and SCH_3, in the 0–6 eV energy range, are displayed in Fig. 2. The measured AE values are given in the diagram of Fig. 3, together with those previously found in the X = I, Br, Cl, $Si(CH_3)_3$ and CH_3 derivatives. Fig. 3 also reports the empty orbital energies (dashed lines) calculated with the MNDO method, shifted by 2 eV to higher energy. Table I compares the energy of the first resonance observed in the ET spectra with the LUMO energy calculated at the MNDO, 3-21G* and 6-31G* * levels in the neutral molecules and with the energy difference between the neutral state and the anion state with the same geometry (ΔSCF, calculated at the 6-31G* * level). The LUMO energy trends predicted by the 3-21G* and 6-31G* * calculations are similar, although according to the latter the energy variations are sizeably reduced. The lowest LUMO energy is calculated for the silicon derivative, while in all the second-row derivatives the LUMO lies at significantly higher energy, in line with the ET data.
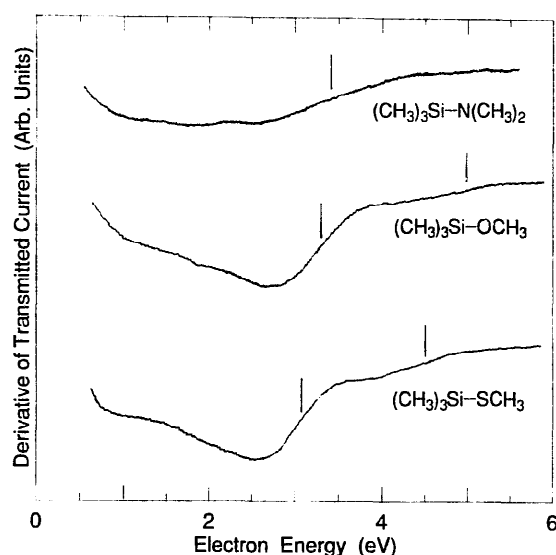

Fig. 2. The derivative of transmitted current as a function of electron energy in gas-phase $(CH_3)_3Si-X$, with $X = N(CH_3)_2$, OCH_3 and SCH_3. Vertical lines locate the most probable attachment energy values.

However, for the chlorine and sulphur derivatives the energy ordering is reversed with respect to experiment. In addition, the LUMO in hexamethyldisilane is predicted to doubly degenerate and to possess mainly Si–C character; in contrast, the ET spectra of linear permethylated polysilanes [6] indicate that the LUMO mainly possesses Si–Si character. The ΔSCF calculations correctly predict the energy of formation of the lowest anion state to be larger for the second-row derivatives than for the sulphur derivative, but fail for the chlorine and silicon derivatives, where anion formation would occur at even higher energy. The semiempirical MNDO
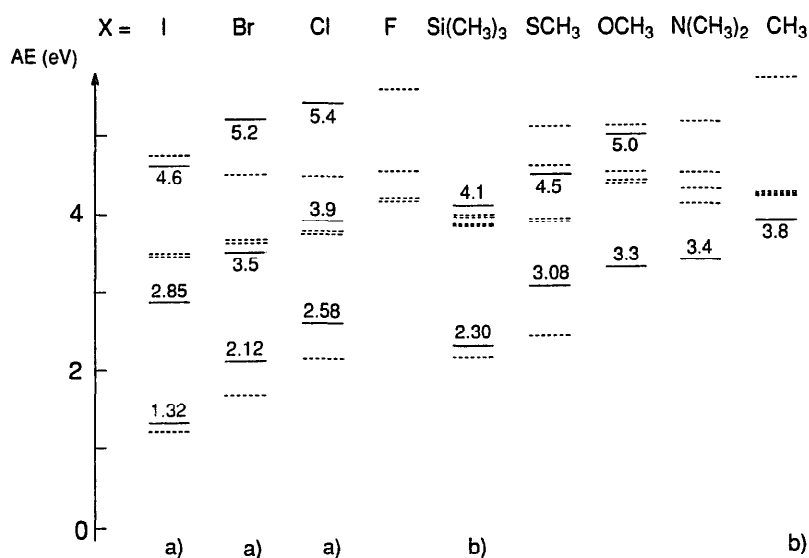

Fig. 3. Correlation diagram illustrating the experimental AE values (continuous lines) and the MNDO empty orbital energies (dashed lines). The calculated energies are shifted by 2 eV to higher energy. (a) Exp. AE values taken from Ref. [8]. (b) Exp. AE values taken from Ref. [6].

Table 1

LUMO energies calculated at the MNDO, 3-21G* and 6-31G** levels, vertical anion/neutral energy differences (ΔSCF) and experimental lowest AEs for the $(CH_3)_3Si-X$ compounds

X	MNDO	3-21G*	6-31G**	ΔSCF	Exp. AE
Cl	0.15	5.46	5.16	5.74	2.58
F	2.15	6.36	5.47	5.26	–
Si(CH₃)₃	0.16	3.21	4.72	5.70	2.30
SCH₃	0.41	5.21	4.84	4.21	3.08
OCH₃	2.37	6.50	5.57	5.49	3.3
N(CH₃)₂	2.12	6.59	5.60	5.53	3.4
CH₃	2.25	6.63	5.55	6.04	3.8

calculations provided a rather good match with the experimental AE trends observed in linear permethylated oligosilanes [6]. Also, in the present series, the experimental trend, at least for the LUMO, is satisfactorily reproduced, even though the calculations tend to overestimate the electron affinity decrease ongoing from the heavier halo derivatives and the disilane to the oxygen and nitrogen derivatives. The MNDO calculations predict the σ* LUMO to possess mainly Si and attached heteroatom character except for X = F and OCH_3, where the LUMO is predicted to possess mainly Si–C character and the σ^*_{Si-X} orbital is calculated to lie at higher energy. In addition, the contribution from the X group to the LUMO becomes less important ongoing from third-row to second-row elements. The best electron acceptor properties are displayed by the I derivative (electron affinity = − 1.32 eV), and within the third-row derivatives, the larger electron affinity is observed for the X = $Si(CH_3)_3$ derivative. There is a gradual electron affinity decrease ongoing from the X = I to the Br and Cl derivatives. For the F derivative, the ET spectrum could not be recorded because the sample is not commercially available; however, the MNDO calculations predict an abrupt electron affinity decrease (about 2 eV) with respect to the Cl analogue, the LUMO energy being calculated at about the same energy as in tetramethylsilane. In addition, the three lowest-lying empty orbitals possess mainly Si–C character, the σ^*_{Si-F} orbital being the fourth LUMO. The MNDO predictions are fully consistent with the ET spectra in the series of the tert-butyl halides [8], where the electron affinity decrease observed ongoing from the chlorine to the fluorine derivative is even larger, clearly indicating that the substituent electronegativity is not the main factor in determining the electron-acceptor properties. In the adiabatic electron affinities calculated by Yoshimura and Tada [11] for the H_3Si-X series, this difference (0.5 eV) betweeen third-row (Cl) and second-row (F) derivatives is strongly attenuated. The experimental AE values measured in the series of the tert-butyl halides as well as in $(CH_3)_3Si-Cl$ were accurately reproduced [8] by MS–Xα calculations, which indicated that the peculiarities of the fluorine derivative are not only concerned

with the high energy of its lowest anion state, but also with its localisation properties. While in tert-butyl chloride (and in the heavier haloderivatives), the lowest-lying anion state was predicted to be more localised on the halogen atom than on the tert-butyl group, the opposite situation was predicted for the fluorine derivative. According to the MS–Xα results, as expected, there is no F 3d contribution in the fluorine derivative, whereas in the chlorine and heavier derivatives, about 50% of the halogen contribution comes from the empty d orbitals. It is to be noted, however, that the stabilising effect of third-row elements has been explained by Yoshimura and Tada [11] without invoking 3d orbital participation. They attributed this effect to: (i) the larger diffuseness in space of the third-row atomic basis functions, with consequent reduction of Coulomb repulsion between the extra electron and the remaining electrons; and (ii) the larger mixing between the silyl group orbitals and third-row substituent orbitals, with consequent delocalisation of the anion SOMO over the entire molecule. It can, in turn, be noted that low-energy empty d orbital participation would imply both the cited effects so that the distinction could assume a formal, rather than physical, meaning. Analogous considerations can of course be made when the oxygen and sulphur derivatives are compared. For the H_3Si-X compounds with X = CH_3, NH_2 and OH, the vertical ionisation potential of the minimum energy geometry ground anion state was calculated [11] to be negative and nearly equal to the adiabatic electron affinity of the neutral molecule. This, in turn, implies that the minimum geometry of the anion state is not too different from that of the neutral parent molecule; in this case, the adiabatic and vertical electron affinity values should also be close to each other (see Fig. 1b). The relatively similar AEs measured here in the oxygen, nitrogen and methyl derivatives are, therefore, in line with the very close adiabatic electron affinity values calculated by Yoshimura and Tada in their corresponding compounds.

4. Calculated neutral state geometries and charge distributions

Table 2 compares some experimental and calculated values of angles and bond distances of interest. For the oxygen, sulphur and nitrogen derivatives, mean values are given. The two sets of calculated data are close to each other. The agreement with available experimental data is slightly better for the 3-21G* values, which will be described in detail. When X is an atom (F, Cl) or a group with a C_3 symmetry axis ($Si(CH_3)_3$, CH_3), the three Si–C bond distances (d_{Si-C}) and the three C–Si–X angles (α) are equal. In the remaining compounds, the molecule is slightly distorted from C_v symmetry. The O–CH₃ or S–CH₃ bonds lie in the pseudo symmetry

Table 2

Selected experimental and theoretical bond distance (Å) and bond angle (°) values in trimethylsilyl derivates, Me_3Si-X

| X		Si–C	Si–X	X–Si–C	C–Si–C
$SiMe_3$	3-21G*	1.897	2.351	110.1	108.8
	6-31G**	1.901	2.371	110.3	108.6
Me	E.D.[a]	1.875	1.875	109.5	109.5
	3-21G*	1.889	1.889	109.5	109.5
	6-31G**	1.893	1.893	109.5	109.5
NMe_2	X-ray[b]	1.863[c]	1.719	110.3[c]	108.7[c]
	E.D.[b]	1.868	1.710	110.3	108.7
	3-21G*	1.887[c]	1.734	110.0[c]	108.9[c]
	6-31G**	1.895[c]	1.739	110.0[c]	109.0[c]
SMe	3-21G*	1.882[c]	2.146	108.4[c]	110.5[c]
	6-31G**	1.890[c]	2.161	108.5[c]	110.4[c]
OMe	3-21G*	1.879[c]	1.641	109.3[c]	109.7[c]
	6-31G**	1.886[c]	1.655	108.6[c]	110.4[c]
Cl	X-ray[d]	1.854[c]	2.091	106.5[c]	112.2[c]
	3-21G*	1.874	2.083	107.2	111.7
	6-31G**	1.878	2.095	107.2	112.0
F	3-21G*	1.868	1.607	107.9	111.1
	6-31G**	1.876	1.610	107.3	111.2

[a] From Ref. [14].
[b] Low temperature (116 K) X-ray diffraction and electron diffraction data from Ref. [15].
[c] Mean values.
[d] Data from the centrosymmetric compound 2,5-dichloro-2,5-dimethyl-2,5-disilahexane, $ClMe_2SiCH_2$-CH_2SiMe_2Cl, from Ref. [16].

plane, which also contains the 'in plane' Si–C bond with unique d and α values (see Scheme 1). In the amino derivative, the geometry at the nitrogen atom is slightly nonplanar (the sum of the angles around nitrogen is 353.2°), the N-bonded methyl groups are distorted from planarity towards the in plane Si-bonded methyl group, in agreement with the crystal and molecular structures [15]. When X = OCH_3 and SCH_3, the unique d_{Si-C} and α values are smaller than those which lie out of the symmetry plane; the distance between the C atoms bonded to the two heteroatoms (C(15)–C(3,5) = 3.65 ± 0.02 Å, see Scheme 1) is not much larger than the sum of the van der Waals radii (3.40 Å). It seems, therefore, that steric hindrance and coulombic repulsion between the methyl groups are reduced by the Si-heteroatom bond bending towards the C(4) atom (that is, by decreasing the 'in plane' α angle), especially for the sulphur derivative, and by an

increase in the bond angle in the oxygen derivative (138.8°, to be compared with 112° in dimethyl ether [14]). In the $N(CH_3)_2$ derivative, the nitrogen lone-pair orbital is perpendicular to the plane containing the Si atom and the C atoms bonded to the nitrogen atom and lies, as well as the in plane Si–C bond, in the plane of pseudo symmetry. The unique d_{Si-C} and α values are in this case larger than the values for the other two Si–C bonds. The C(3)–C(15) and C(4)–C(16) distances (3.330 and 3.327 Å, respectively) are smaller than the sum of the van der Waals radii, even though all the distances between H atoms are larger than the sum of their van der Waals radii. This hindered conformation, where quasi planarity at the nitrogen atom increases the p character of the N_{1p} orbital, is favoured by an increase in the stabilising charge-transfer N_{1p}/σ^*_{SiC} interaction. Comparison between calculated and experimental d_{Si-C} and d_{Si-X} bond lengths (see Table 2) shows that the 3-21G* values are about 0.02 Å larger than those obtained by X-ray diffraction or electron diffraction. The only exception is d_{Si-Cl}, calculated to be 0.01 Å shorter with respect to the experimental value (2.091 Å) found [16] in 2,5-dichloro-2,5-dimethyl-2,5-disilahexane, $(ClSi(CH_3)_2CH_2)_2$. In Ph_3Si–Cl, however, this distance was found [17] to be only 2.074 Å or 2.080 Å. Bond angles are also reproduced with good accuracy. The calculated trends in bond lengths and angles thus appear to be significant. The calculated d_{Si-C} value gradually decreases with X in the order: $Si(CH_3)_3 >$ $CH_3 > N(CH_3)_2 > SCH_3 > OCH_3 > Cl > F$. This trend seems to be significantly affected by the inductive electron-withdrawing effect of the substituent and the consequent electron demand along the σ skeleton. It is interesting to note that the C–Si–X (α) angles roughly decrease in the same direction, but with some inversions: $Si(CH_3)_3 > N(CH_3)_2 > CH_3 > OCH_3 > SCH_3$ $> F > Cl$. In particular, in the third-row S and Cl derivatives, α is smaller (that is, the Si–C bonds are closer to the X substituent) than in the corresponding second-row O and F derivatives. This finding could be correlated to mesomeric electron-acceptor properties of third-row substituents, that is, to a stabilising effect of mixing of the filled $\sigma_\pi(SiC_3)$ orbitals with low-energy empty orbitals of the substituent. While in the sulphur derivative, the empty orbital involved could be a σ^*_{S-C}
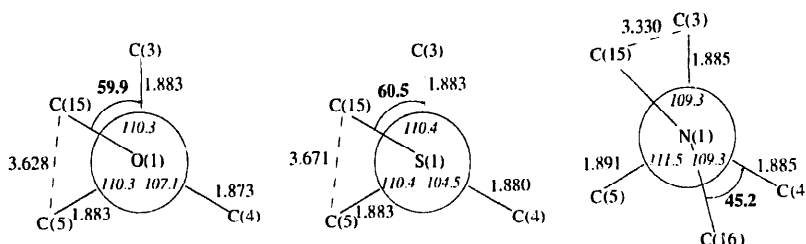
Scheme 1.

Table 3

Relative charge (e) at the Me_3, Si and X groups or atoms of the Me_3SiX derivatives with respect to Me_3SiMe, obtained by 6-31G** calculations[a]

X	Δq_{Me_3}	Δq_{Si}	Δq_X
NMe_2	−0.036	+0.148	−0.112
OMe	−0.009	+0.173	−0.164
SMe	+0.078	−0.055	−0.024
Cl	+0.158	−0.028	−0.130
F	+0.050	+0.171	−0.221
$[SiMe_3$	+0.008	−0.288	+0.280]

[a]A negative value indicates an increase of negative charge with respect to the corresponding group or atom in the reference compound (Me_3SiMe: Me_3 = −0.840, Si = +1.120, Me = −0.280 e).

orbital, in the chlorine derivative, it would be necessary to invoke $3d$ orbitals for symmetry reasons. On the other hand, according to the results of MS–Xα calculations [18], the low-lying σ^* orbitals in thioderivatives possess large S $3d$ character. To obtain more information on this point and on the possible effects on the charge distributions, the electronic charges localised at the $(CH_3)_3$, Si and X fragments which constitute the molecules were analysed. The 6-31G** results are displayed in Table 3. Similar trends, but with larger charge separations, are found at the 3-21G* level. The reported Δq values are relative to the charge distribution calculated in the reference molecule tetramethylsilane: $(CH_3)_3$ = −0.840, Si = +1.120, CH_3 = −0.280 e. Replacement of the methyl substituent with the more electronegative $N(CH_3)_2$ group causes a shift of negative charge from the silicon atom to the X substituent. However, an increase in negative charge is also calculated at the silicon-bonded methyl groups while, of course, the silicon atom becomes significantly more positive. This result is consistent with the above-mentioned lone pair to σ^*_{SiC} back donation. The only other substituent which displays such behaviour (increase of negative charge on the methyl groups and of positive charge on the silicon atom) is OCH_3. The remaining second-row substituent, fluorine, is even more electronegative and with less propension to mesomeric donation than oxygen, so that it attracts negative charge from all the molecule. A large increase of negative charge (Δq = −0.130 e) at the substituent also occurs when X = Cl, but with a concomitant increase of negative charge at the silicon atom, at the expense of the methyl groups (Δq = +0.158 e). This positive charge shift at the methyl groups, three times as large as that predicted when X is the more electronegative fluorine atom, together with the enlargement of the base of the SiC_3 pyramid noted above, is consistent with mesomeric donation from the filled Si–C orbitals towards chlorine empty $3d$ orbitals. Finally, excluding the particular case of X = $Si(CH_3)_3$ where the substituent is

equal to the remaining part of the molecule, a small increase of negative charge (Δq = −0.024 e) at the substituent is found for the replacement of a methyl group with an SCH_3 group. The sulphur atom is, in fact, the least electronegative and most polarizable among the heteroatoms considered here. Nevertheless, the effect produced on the silicon-bonded methyl groups (Δq = +0.078 e) is larger than that due to the fluorine atom, again in line with mesomeric back donation to low-lying empty orbitals of substituents containing third-row elements.

Acknowledgements

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