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Molecular Structure of 1-Isothiocyanatosilatrane: Ab Initio and DFT Calculations

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Introduction

Previous X-ray studies[1−6] on silatranes, $RSi(OCH_2CH_2)_3N$, have shown that they have an approximate C_3 symmetry and the geometry around the silicon atom looks rather pentacoordinate via a transannular dative bond between silicon and nitrogen atoms. The presence of a transannular Si−N bond in silatranes can be explained by the fact that the nitrogen atom might donate its lone-pair electrons to the silicon atom. It is a general consensus from accumulated experimental results that more electronegative substituents R, such as fluorine and chlorine, usually help to form shorter Si−N bond distances.[7] In addition, the length of the Si−N bond is significantly dependent on such physical environments of a molecule as the solid state and the gas phase. It can be generally expected that the crystal-packing forces make the molecular geometry in the solid state to be somewhat different from that in the gas phase. Previous electron diffraction (ED) studies[8,9] on silatranes have also found that they have generally longer Si−N distances in the gas phase rather than in the solid state. However, no experimental studies for molecules in the gas phase other than 1-methylsilatrane and 1-fluorosilatrane have been performed to date, so the precise relationship between the electronic nature of the substituents and the Si−N distances for silatranes in the gas phase are not clearly understood yet.

In this paper, ab initio and density functional theory (DFT) methods are applied to examine the precise molecular structure of the 1-isothiocyanatosilatrane, $SCNSi(OCH_2CH_2)_3N$, in which the nitrogen atom of the ligand NCS^- is directly connected to the Si atom. We compare its computed geometrical parameters with available X-ray crystal structure data and crystal structures of its analogues with different substituents such as F and Cl. We also compare its computed isotropic ^{13}C, ^{15}N, and ^{29}Si magnetic shielding constants using the gauge-including atomic orbital (GIAO) method[10] with the available experimental NMR data. Finally, we discuss the characteristics of the transannular Si−N bond of this molecule by population analysis.

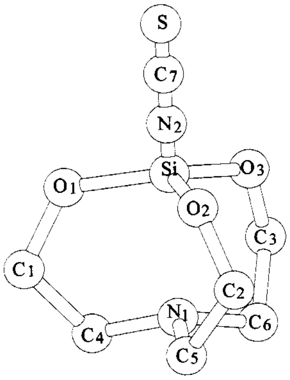

Figure 1. Molecular structure of 1-isothiocyanatosilatrane with atomic numbering (hydrogen atoms are omitted for clarity).

Computational Details

All ab initio and density functional theory calculations are performed using the Gaussian 94 program.[11] The molecular geometry of 1-isothiocyanatosilatrane is optimized at both the restricted Hartree−Fock (RHF) and Becke's three-parameter-hybrid (B3LYP)[12−14] levels with 6-31+G* and 6-311G* basis sets. To make a more intensive comparison between molecular structures of this molecule and its analogues, we have also performed the geometry optimizations for 1-fluorosilatrane and 1-chlorosilatrane at the B3LYP/6-31+G* level.

Results and Discussion

Molecular Structure of 1-Isothiocyanatosilatrane. The molecular structure of 1-isothiocyanatosilatrane is illustrated in Figure 1 along with the atomic numbering. It can be assumed that there are two possible isomers, so-called endo and exo forms, according to whether lone-pair electrons of the transannular nitrogen atom N_1 point toward the silicon atom or not. A few ab initio studies[15,16] have actually reported both exo and endo forms in some analogous systems such as azaphosphatranes. In substituted silatranes, however, there are no experimental or ab initio reports about the existence of exo forms, even though previous semiempirical studies[17−19] predicted the existence of the exo forms of silatranes. Moreover, recent ab

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Table 1. Geometrical Parameters for 1-Isothiocyanatosilatrane at the RHF and B3LYP Levels

	RHF		B3LYP		
parameters	6-31+G*	6-311G*	6-31+G*	6-311G*	exptl[a]
		Bond Lengths (Å)			
$r(Si-N_1)$	2.454	2.484	2.327	2.353	2.007(3)
$r(Si-O_1)$	1.634	1.628	1.672	1.665	1.637(2)
$r(O_1-C_1)$	1.399	1.398	1.414	1.413	1.429(4)
$r(C_1-C_4)$	1.527	1.527	1.535	1.534	1.510(6)
$r(C_4-N_1)$	1.454	1.453	1.471	1.469	1.484(4)
$r(N_2-C_7)$	1.160	1.157	1.189	1.184	1.160(4)
$r(C_7-S)$	1.600	1.596	1.596	1.593	1.594(3)
$r(Si-N_2)$	1.736	1.731	1.739	1.739	1.800(3)
		Bond Angles (deg)			
$\angle SiO_1C_1$	125.0	125.6	122.9	123.4	119.7(2)
$\angle O_1SiO_2$	116.0	115.6	117.8	117.5	120.6(1)
$\angle O_1C_1C_4$	109.7	109.7	109.7	109.8	108.2(3)
$\angle C_1C_4N_1$	108.0	107.8	107.3	107.2	105.6(3)
$\angle N_2SiO_1$	101.7	102.3	98.7	99.0	92.2(1)

[a] Reference 5.

initio vibrational frequency analyses for some silatranes have revealed that the exo forms are not at local minima.[20]

The optimized geometrical parameters of 1-isothiocyanatosilatrane at various levels of theory are summarized in Table 1 along with data of the X-ray crystallography.[5] From the results of the previous X-ray experiment, the bond angle $\angle SiN_2C_7$ in the solid state deviates somewhat from 180°. This means there is no principal axis of rotation for the experimental structure of this molecule. In this theoretical study, however, the bond angle $\angle SiN_2C_7$ in the gas phase is found to be around 180° at the RHF/6-31G* level, so this angle is held to be 180° during geometry optimizations so as to keep at least C_3 molecular symmetry of 1-isothiocyanatosilatrane. The vibrational frequency calculations at the RHF/6-31G* level show that a final optimized geometry is at a real minimum point on the potential energy surface. This fact supports that C_3 symmetrical constraint is sufficient to understand the bonding nature of this molecule compared with that of other substituted silatranes.

Some parameters obtained from this study differ rather markedly from those obtained in the X-ray crystallographic determination. The most drastic difference is the distance between Si and the transannular nitrogen atom. In the Si−O bond length, the computed values at the RHF levels are closer to the experimental value of 1.637(2) Å. However, this bond length is sensitively affected by adding the electron correlation effect at the B3LYP levels. The computed value of this bond length is about 1.67 Å at the B3LYP/6-31+G* level. One can find a slight decrease of the Si−O bond length when the triple split valence basis set is taken into account at the B3LYP/6-311G* level. On the other hand, the computed O_1-C_1 bond lengths at both RHF and B3LYP levels are somewhat shorter than the X-ray value. This unusual result might be because of either the crystal packing forces in the solid state or an experimental unreliability.

The $Si-N_1$ bond length is the most important geometrical parameter in examining the structures of substituted silatranes. In the present study, this computed bond length shows somewhat characteristic behavior. The $Si-N_1$ bond distances computed at the RHF levels are considerably longer than those at the B3LYP levels where the electron correlation effects are considered, which is contrary to our expectation. It is also shown that the computed bond lengths slightly increase as the basis size is increased at both the RHF and B3LYP levels. The computed value of 2.327 Å at the B3LYP/6-31+G* level is quite a bit longer than the experimental bond length of 2.007(3) Å measured in the solid state.

Table 2. Molecular Parameters Connected with the Si Atom (Distances, Å; Angles, deg) and NMR Chemical Shifts (ppm) of R-Substituted Silatrane

	R = F[a]			R = Cl[b]	
parameter	B3LYP/ 6-31+G*	gas	crystal	B3LYP/ 6-31+G*	crystal
$r(Si-N)$	2.358	2.32(1)	2.042(1)	2.452	2.023
$r(Si-R)$	1.620	1.568(6)	1.622(1)	2.082	2.153
$\angle OSiO$	117.5	117.8(1)	119.6(2)	116.5	
$\angle RSiO$	99.2	98.7(3)	93.8(2)	100.9	93.4
^{29}Si			−100.4		−85.2
$^{15}N^c$			−348.3		−348.1

[a] Reference 9. [b] Reference 6. [c] Transannular nitrogen.

At this stage of discussion, it is very meaningful to compare the experimental molecular parameters among R-substituted silatranes (R = F, Cl) in order to infer the molecular geometrical parameters of 1-isothiocyanatosilatrane in the gas phase. In general, the ligand NCS^- behaves chemically very much like halide ions, and its similarities to the halogens appear also in the basic properties. Although the ligand NCS^- is ambidentate, NCS^- (N donor) in particular is classified as a borderline base as Br^-. It can behave reasonably as a hard base by coordination via a hard nitrogen atom. As such, it tends to resemble fluorine or chlorine considerably more than bromine.[21] In Table 2 are shown experimental molecular parameters and chemical shifts of R-substituted silatranes (R = F, Cl).[6,9] The computed $Si-N_1$ bond distance of ~2.33 Å at the B3LYP/6-31+G* level for 1-isothiocyanatosilatrane is very close to the experimental value 2.324(14) Å of 1-fluorosilatrane[9] despite a different substituted ligand.

The bond angle around the Si atom, such as $\angle N_2SiO_1$, is also an important factor to judge how much the geometry around the Si atom deviates from a pentacoordinated trigonal bipyramidal structure. This bond angle is computed to be about 98° at the B3LYP levels, which is compared with $\angle FSiO$ of 98° for 1-fluorosilatrane in the gas phase, while the X-ray value is about 2° away from 90°, corresponding to a regular trigonal bipyramid. This means that crystal-packing forces might assist this molecule to make some kind of bond between nitrogen and silicon atoms in the solid state. This effect causes the geometry around the silicon atom to have five rather than four coordinations in the solid state. The present study shows that the molecular geometry around the Si atom in the gas phase is somewhat distorted from the ideal trigonal bipyramid toward the tetrahedron with four coordinations.

In contrast with the $Si-N_1$ distance, the computed axial $Si-N_2$ bond lengths at all levels are shorter than the experimental values in the crystal. Because the Si−F bond length of 1-fluorosilatrane in the gas phase is shorter than that in the solid state, it cannot be unreasonable to conclude that the $Si-N_2$ bond length of 1-isothiocyanatosilatrane in the gas phase should be considerably shorter than that in the crystal. Hence, the computed values at all levels, which are significantly shorter than the X-ray value, might be close to the bond length in the gas phase. It is very interesting that geometrical parameters around the Si atom are well related to the distortion of the axial N_1 atom from the trigonal bipyramidal structure. The reason why the axial $Si-N_2$ bond length in the gas phase is shorter

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than that in the solid state is explained by the enlargement of the axial Si$-$N$_1$ bond on the opposite side because the bonding in the silatranes is best described as a dative Si$-$N bond but with sufficient three-center interaction to produce a slight enlargement of the Si$-$R bond. This means that the lengthening of one axial bond in a regular trigonal bipyramid might cause the other axial bond to be contracted a little. Hence, the overall geometry around the Si atom of 1-isothiocyanatosilatrane is somewhere between a trigonal bipyramid and a tetrahedron.

Taking a look at the molecular parameters for the R-substituted silatranes in Table 2, we also see discrepancies between some parameters around the Si atom for both gas and solid phases. It seems to us that the computed parameters at the B3LYP/6-31+G* level would be likely to be closer to the gas-phase structure of each silatrane. Thus, in 1-fluorosilatrane and 1-chlorosilatrane, there appears to be a nitrogen$-$silicon dative bond in the crystal, whereas in the gas phase, the Si$-$N separation is very large, suggesting a much weaker interaction. Perhaps intermolecular interactions might compress the molecule in the crystal to facilitate the formation of an Si$-$N bond. If one looks at both $\angle$OSiO and $\angle$RSiO in the gas phase as well as in the crystal, the gas-phase geometry may be considered to be distorted tetrahedral, while the crystal-phase structure is distorted trigonal bipyramidal. The same is true for 1-isothiocyanatosilatrane.

Another important factor is the relation between the Si$-$N$_1$ bond length and the electronic behavior of a substituent, which should be examined, in R-substituted silatranes. It is well-known from previous results that the Si$-$N$_1$ bond length in a silatrane decreases as an electronegative substituent becomes more strongly bound to the Si atom. Nevertheless, the reason why the shortest bond between Si and N occurs in 1-chlorosilatrane among several silatranes was explained by the difference of leaving-group ability between Cl and F atoms.[22] According to the X-ray diffraction results, the bond length between Si and N$_1$ of 1-isothiocyanatosilatrane is somewhat shorter than that of 1-fluorosilatrane and 1-chlorosilatrane, as can be seen in Tables 1 and 2. In general, the isothiocyanato group NCS is considered to be both electron-withdrawing via an inductive effect and electron-donating via a resonance effect. This dualism of the isothiocyanato group is caused by the behavior of the lone-pair electrons on its nitrogen atom. Actually, it is possible that these lone-pair electrons can attack both silicon and carbon atoms. If they attack the silicon atom, the NCS group acts as the electron-donating group via the resonance effect because of the $p_\pi-d_\pi$ interaction between the nonbonding pair of electrons on N and the vacant d_π orbitals on Si. At the same time, because the polarizability of this group can increase remarkably when the lone pair of nitrogen attacks the back side carbon atom, this group also has electron-donating behavior via an inductive effect. Thus, comparing the Si$-$N$_1$ bond length in this 1-isothiocyanatosilatrane with that of its analogues might be a clue to understand how the NCS group functions in this molecule.

In this isothiocyanatosilatrane, structural features such as a significantly shorter Si$-$N$_2$ bond may suggest that the NCS group has only a little predominance of electron withdrawing over electron donation. Therefore, one can infer that the electron-withdrawing effect of the NSC group can be compared to that of F or Cl. The computed Si$-$N$_1$ distance of 2.327 Å at the B3LYP/6-31+G* level is somewhat shorter than that of 1-fluorosilatrane or that of 1-chlorosilatrane at the same level of theory. This also supports the fact that the electron-withdrawing ability of the NCS group is as large as that of fluorine or chlorine.

Table 3. Calculated NMR Chemical Shifts (ppm) for 1-Isothiocyanatosilatrane at the RHF and B3LYP Levels Using the B3LYP/6-31+G* Optimized Geometry

calculational level	Si	N$_1$	N$_2$	C$_1$	C$_4$	C$_7$
RHF/6-31+G*	−84.7	−466.7	−363.9	53.5	50.4	150.8
RHF/6-311G*	−98.3	−487.6	−380.9	54.3	49.4	161.0
RHF/6-311+G*	−98.0	−492.7	−386.2	54.8	49.6	163.5
B3LYP/6-31+G*	−85.7	−341.2	−264.6	60.2	54.3	129.8
B3LYP/6-311G*	−104.3	−361.0	−280.0	61.8	55.8	141.8
B3LYP/6-311+G*	−104.5	−367.9	−286.3	62.0	55.8	144.3
exptl[a]	−103.0	−347[b]	−247.8	58.8	52.5	133.8

[a] Reference 5. [b] Predicted by the equation $r(\mathrm{Si-N}) = -4.30 - [(1.82 \pm 0.08) \times 10^{-2}]\delta(^{15}\mathrm{N})$.[23]

It is quite interesting that the magnitude of the difference in the Si$-$N$_1$ dative bond lengths between these two halosilatranes in the gas phase is reversed in the solid state. As can be seen in Table 2, the computed Si$-$N$_1$ bond length of 1-fluorosilatrane is somewhat shorter than that of 1-chlorosilatrane. This means that the electronegativities of these two halogens as it stands affect this bond length significantly. Therefore, one can surmise from these facts that the bond length of the Si$-$N dative bond in the gas phase might be rarely affected by the leaving-group ability of the substituent, whereas the length of this bond in the solid state is somewhat influenced by the leaving-group ability.

Isotropic Chemical Shifts and Population Analyses. In studies of substituted silatranes, NMR isotropic shielding tensors are very useful parameters in examining molecular structures as well as the electronic behaviors of substituents in those compounds. Both experimental and theoretical NMR chemical shifts for 1-isothiocyanatosilatrane are summarized in Table 3. As can be seen in this table, the computed ^{29}Si NMR chemical shifts at both B3LYP/6-311G*//B3LYP/6-31+G* and B3LYP/6-311+G*//B3LYP/6-31+G* levels are in excellent agreement with the experimental value.[12] Because there is no available experimental ^{15}N NMR chemical shift of the N$_1$ atom either in solution or in the solid phase for this molecule, we have predicted the ^{15}N NMR chemical shift of the transannular nitrogen for 1-isothiocyanatosilatrane in the crystal by using an empirical equation, $r(\mathrm{Si-N}) = -4.30 - [(1.82 \pm 0.08) \times 10^{-2}]\delta(^{15}\mathrm{N})$.[2,23] The predicted chemical shift is around −347 ppm, which is likely to be very close to the experimental value because these isotropic ^{15}N chemical shifts for halosilatranes, including this value, do not show pronounced variation upon the change of substituents, as can be seen in Table 2. The computed ^{15}N chemical shifts for N$_1$ and N$_2$ atoms at the B3LYP levels are in good agreement with the predicted value of −347 ppm and the measured value of −247.8 ppm, respectively. The results tell us that the electronic environment around the N$_1$ atom in the halogen-substituted silatranes is scarcely affected by the transannular Si$-$N$_1$ bond, even though this bond length and ^{29}Si are quite sensitive to the change of substituents (see Table 2). On the other hand, ^{13}C NMR chemical shifts for carbon nuclei C$_1$, C$_4$, and C$_7$ are in good agreement with those of experiments at the B3LYP levels rather than at the RHF levels.

To see the bonding property of the Si$-$N$_1$ bond for R-substituted silatranes, we have calculated charges and bond orders by using natural population analysis as well as traditional Mulliken analysis. The computed atomic charges for R-

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(23) The dependence of ^{15}N NMR chemical shifts $\delta(^{15}\mathrm{N})$ on the bond lengths $r(\mathrm{Si-N})$ in 1-substituted silatranes in the solid, solution, and vapor states. See ref 2.

Table 4. Total Atomic Charges for R-Substituted Silatranes at the RHF/6-31G*//B3LYP/6-31G* Level

atom	R = F	R = Cl	R = NCS
Si	2.67	2.45	2.60
O_1	−1.01	−1.02	−1.00
C_1	−0.03	−0.03	−0.03
C_4	−0.23	−0.23	−0.23
N_1	−0.66	−0.65	−0.66

substituted silatranes (R = F, Cl, NCS) by natural population analysis are summarized in Table 4. Among many atoms in silatranes, the silicon atom is directly influenced by the electronic nature of a substituent. As can be seen in Table 4, the silicon atom in 1-fluorosilatrane has a slightly larger positive charge than silicon atoms in other silatranes. This means that the electron-withdrawing effect of the fluorine atom is rather strong among these three molecules and/or the strength of the Si−N dative bond for this compound is somewhat weaker than those of others. According to the Mulliken overlap population analysis, the computed bond order of 1-fluorosilatrane is somewhat smaller than those of others, which is well consistent with our justification.

On the other hand, the charge on the N_1 atom can provide an insight into the nature of the Si−N bond. The magnitudes of the negative charge of the N_1 atom are much the same for these three compounds. This means that the ability of electron donation from N_1 to Si upon a change of substituents is not crucial to understand the nature of the Si−N_1 bond. The computed charges for other atoms, such as O_1, C_1, and C_4, are rarely dependent upon a change of the substituents. This fact is also consistent with the results of isotropic chemical shifts, which are discussed above.

Conclusion

The molecular structure of 1-isothiocyanatosilatrane is intensively investigated with both ab initio and DFT methods. The computed molecular structures at the B3LYP levels in Table 1, which should reproduce gas-phase experiments, can explain the structural behavior of this molecule in the gas phase. Most of the computed parameters compare favorably with those obtained for other related molecules in the gas phase. Some of the computed structural properties are quite different from those found by experiments in the solid state. In particular, the computed transannular Si−N bond length at the B3LYP levels is about 0.3 Å longer than the experimental distance by X-ray diffraction. However, this value can be reasonably compared with the available electron diffraction value for 1-fluorosilatrane. On the contrary, the computed Si−N_2 bond length, which is on the opposite side of the transannular Si−N_1 bond, is somewhat longer than the experimental value in the solid state. This result is well related to the fact that the lengthening of the transannular Si−N_1 bond would affect the bond length of the opposite axial Si−N_2 bond.

In addition, computed isotropic chemical shifts for ^{29}Si, ^{15}N, and ^{13}C nuclei in 1-isothiocyanatosilatrane at the B3LYP levels are in reasonable agreement with experimental values. Considering the ^{29}Si and ^{15}N NMR chemical shifts in Tables 2 and 3, it can be said that there are some similarities in the electronic environments between 1-fluorosilatrane and 1-isothiocyanatosilatrane. This fact convinces us that the computed molecular structures at the B3LYP/6-31+G* level of 1-isothiocyanatosilatrane, which are similar to the gas-phase geometry of 1-fluorosilatrane, should be close to the true molecular geometry in the gas phase.

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