

Ab initio molecular orbital investigation of SiOH^+-XH , SiOH^+-X_2 and $\text{SiOH}^+-\text{XY}(\text{YX})$ ($\text{X} = \text{Y} = \text{F}, \text{Cl}$ and Br) proton-bond complexes

Mohammad Solimannejad^{a,*}, Masoud Haratian^a, Abderrahim Boutalib^b

^a Quantum Chemistry Group, Department of Chemistry, Arak University, 38156-879 Arak, Iran

^b Département de Chimie, Université Cadi Ayyad, Faculté des Sciences Semlalia, B.P. 2390 Marrakech, Morocco

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Abstract

The results of theoretical studies on structures and energetics are presented for proton-bond complexes SiOH^+-XH , SiOH^+-X_2 and $\text{SiOH}^+-\text{XY}(\text{YX})$ ($\text{X} = \text{Y} = \text{F}, \text{Cl}$ and Br). In all the monocations complexes, the halogen atom shares a proton with SiO . The calculated energetic results show that the stability decreases when descending in the corresponding periodic table column. The possible proton transfer dissociation processes of $\text{SiOH}^+ + \text{XH}$, $\text{SiOH}^+ + \text{X}_2$ and $\text{SiOH}^+ + \text{XY}$ systems into XH_2^+ , X_2H^+ , XYH^+ and YXH^+ , and SiO are calculated to be endothermic. The natural bond orbital (NBO) results show that the largest intermolecular charge transfer is found in the Br bonded complexes.

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1. Introduction

Proton-bond complexes are long been known as intermediates of proton transfer reactions, which are important in physical, chemical and biological properties and processes. Accurate knowledge of the thermodynamics, reactivity and mechanism of complexation and dissociative proton transfer reactions would serve as a useful framework. Numerous experimental and theoretical studies have been devoted to this type of compounds concerning their structural parameters, the nature of the reaction intermediates [1–21]. On the other hand, Bohme and co-workers have extensively studied the gas-phase reactions of Si^+ and SiOH^+ with small molecules. They provide insight of the chemical bonding of silicon with hydrogen, carbon, nitrogen, oxygen and sulfur [22–25]. Recently, Dopfer and co-workers have reported about the infrared photodissociation spectra and

molecular structures of SiOH^+-X ($\text{X} = \text{He}, \text{Ne}, \text{Ar}, \text{N}_2$) and $\text{SiOH}^+-\text{Ar}_n$ ($n = 1-10$) ionic hydrogen complexes [26,27]. They have showed that experimentally and theoretically, all studied complexes prefer linear configurations. More recently we reported theoretical studies on structures and energetics for proton-bond complexes $\text{N}_2\text{H}^+-\text{XH}$, $\text{N}_2\text{H}^+-\text{X}_2$ and $\text{N}_2\text{H}^+-\text{XY}(\text{YX})$ ($\text{X} = \text{Y} = \text{F}, \text{Cl}$ and Br) at the B3LYP/6-311++G(3df,3pd) level of theory [28]. We have shown that in all the monocations complexes, the halogen atom shares a proton with N_2 . We have also shown that the stability decreases when descending in the corresponding periodic table column and the possible proton transfer dissociation processes of $\text{N}_2\text{H}^+ + \text{XH}$, $\text{N}_2\text{H}^+ + \text{X}_2$ and $\text{N}_2\text{H}^+ + \text{XY}$ systems into XH_2^+ , X_2H^+ , XYH^+ and YXH^+ and molecular N_2 are endothermic. In this paper, we report our investigation on the SiOH^+-HX , SiOH^+-X_2 and $\text{SiOH}^+-\text{XY}(\text{YX})$ ($\text{X} = \text{Y} = \text{F}, \text{Cl}$ and Br) complexes. The possible proton transfer dissociation processes of $\text{SiOH}^+ + \text{XH}$, $\text{SiOH}^+ + \text{X}_2$ and $\text{SiOH}^+ + \text{XY}$ systems into XH_2^+ , X_2H^+ , XYH^+ and YXH^+ , and SiO are examined. To our knowledge, no comparative ab initio studies of these complexes have been carried out up to

* Corresponding author. Tel.: +98 861 2777401; fax: +98 861 2774031.
E-mail address: m-solimannejad@araku.ac.ir (M. Solimannejad).

now. The electronic structure of these complexes has been analyzed and the relative stabilities are examined.

2. Computational details

Calculations were performed using the GAUSSIAN98 program system [29]. The geometry optimizations and frequency calculations were performed at the MP2(full)/6-31++G(d,p) level. Harmonic vibrational frequency calculations were performed to confirm whether the predicted structure is a minimum and to evaluate zero-point vibrational energies (ZPE) corrections. The ZPE corrections are obtained from scaled MP2(full)/6-31++G(d,p) frequencies (scaled by the factor 0.96) [30]. Final energies were calculated at the QCISD(T)/6-31++G(d,p)/MP2(full)/6-31++G(d,p) + ZPE level. The charge distribution in the complexes has been analyzed from the natural bond orbital (NBO) [31] partitioning scheme at the MP2(full)/6-31++G(d,p) level. Atomic populations obtained from this analysis are fewer bases set dependent than those corresponding to the Mulliken population analysis [31].

3. Results and discussion

Association of SiOH^+ ($C_{\infty v}$ symmetry) with HX , X_2 and XY leads to C_s symmetry monocation complexes SiOH^+-XH , SiOH^+-X_2 , SiOH^+-XY and SiOH^+-YX that was calculated to be a stable structure at the MP2(full)/6-31++G(d,p) level of theory. No symmetry constraints were imposed during the optimization process and the geometry searches were carried out for a number of possible isomers to ensure the location of the global minimum. For the association of SiOH^+ with FH , we have found two stable conformations: the conformation where the halogen atom shares a proton with SiO and the $\text{HF}-\text{SiOH}^+$ conformation where the halogen atom is bonded to Si atom. The SiOH^+-FH conformation is the more stable at the QCISD(T)/6-31++G(d,p)/MP2(full)/6-31++G(d,p) + ZPE level. For the SiOH^+-ClF and SiOH^+-BrF complexes, the optimization leads to SiOH^+-FCl and SiOH^+-FBr , respectively. Tables 1–3 list the most important optimized geometrical parameters of SiOH^+-XH , SiOH^+-X_2 and $\text{SiOH}^+-\text{XY}(\text{YX})$ ($\text{X} = \text{Y} = \text{F}, \text{Cl}$ and Br) complexes, respectively. Tables 4 and 5 list the MP2(full)/6-31++G(d,p) unscaled vibrational frequencies of all investigated complexes along with the corresponding SiOH^+ monomer values. In Table 6 we reported the calculated association energies of SiOH^+ with HX , X_2 and $\text{XY}(\text{YX})$. We also reported in Table 6 the calculated NBO–MP2(full)/6-31++G(d,p) charge transfer from HX , X_2 and $\text{XY}(\text{YX})$ moieties to SiOH^+ . Table 7 lists the energy for the proton transfer dissociation process of $\text{SiOH}^+ + \text{XH}$, $\text{SiOH}^+ + \text{X}_2$ and $\text{SiOH}^+ + \text{XY}(\text{YX})$ systems into XH_2^+ , X_2H^+ , XYH^+ and YXH^+ , and SiO .

Table 1
MP2(full)/6-31++G(d,p) optimized bond lengths (Å) and bond angles (°) of SiOH^+-XH complexes ($\text{X} = \text{F}, \text{Cl}$ and Br)^a

Compound	Si–O	O–H ⁺	H ⁺ –X	X–H	∠H ⁺ –X–H
SiOHFH^+	1.554	0.991	1.576	0.935	135.2
FH_2^+			0.969	0.969	113.2
FH				0.926	
SiOHClH^+	1.556	0.996	2.006	1.275	106.2
ClH_2^+			1.293	1.293	95.7
ClH				1.281	
SiOHBrH^+	1.555	1.005	2.074	1.440	98.5
BrH_2^+			1.430	1.430	93.2
BrH				1.406	

^a The optimized O–Si and O–H⁺ in SiOH^+ ion are 1.574 and 0.98 Å, respectively.

Table 2
MP2(full)/6-31++G(d,p) optimized bond lengths (Å) and bond Angles (°) of SiOH^+-X_2 complexes ($\text{X} = \text{F}, \text{Cl}$ and Br)

Compound	Si–O	O–H ⁺	H ⁺ –X	X–X	∠H ⁺ –X–X
SiOHF_2^+	1.558	0.986	1.810	1.437	98.6
F_2H^+			0.999	1.440	100.9
F_2				1.433	
SiOHCl_2^+	1.557	0.992	2.030	2.023	99.6
Cl_2H^+			1.298	2.032	99.6
Cl_2				2.019	
SiOHBr_2^+	1.555	1.002	2.087	2.313	91.2
Br_2H^+			1.433	2.315	96.6
Br_2				2.313	

In the SiOH^+-XH ($\text{X} = \text{F}, \text{Cl}$ and Br) complexes, the halogen atom shares a proton with SiO and weakens the H^+-O bond strength. Consequently, the H^+-O bond length becomes longer than in the isolated SiOH^+ ion. Indeed, the MP2(full)/6-31++G(d,p)-level-calculated H^+-O distance in the free SiOH^+ ion is 0.975 Å. The calculated H^+-O bond lengths are elongates to 0.991, 0.996 and 1.005 Å in the SiOH^+-FH , SiOH^+-ClH and SiOH^+-BrH complexes, respectively. Thus the lengthening of the H^+-O bond is the major effects of complexation on the SiOH^+ properties and

Table 3
MP2(full)/6-31++G(d,p) optimized bond lengths (Å) and bond angles (°) of $\text{SiOH}^+-\text{XY}(\text{YX})$ complexes ($\text{X} = \text{Y} = \text{F}, \text{Cl}$ and Br)

Compound	Si–O	O–H ⁺	H ⁺ –X (Y)	X–Y	∠H ⁺ –X–Y or ∠H ⁺ –Y–X
SiOHFCI^+	1.556	0.990	1.597	1.691	123.7
ClFH^+			0.968	1.787	112.2
FCl				1.667	
SiOHFBr^+	1.555	0.995	1.547	1.821	133.2
BrFH^+			0.962	1.941	114.1
BrF				1.793	
SiOHClBr^+	1.556	0.995	2.000	2.175	97.1
BrClH^+			1.295	2.202	98.3
BrCl				2.163	
SiOHBrCl^+	1.556	1.000	2.095	2.163	93.4
ClBrH^+			1.434	2.150	97.0

Table 4
MP2(full)/6-31++G(d,p) unscaled vibrational frequencies (cm^{-1}) of $\text{SiOH}^+-\text{XH}(\text{X}_2)$ complexes ($\text{X} = \text{F}, \text{Cl}$ and Br)^a

Frequency	SiOHFH^+	SiOHClH^+	SiOHBrH^+	SiOHF_2^+	SiOHCl_2^+	SiOHBr_2^+
ω_1	110 (18)	101 (21)	137 (15)	51 (3)	41 (4)	33 (5)
ω_2	128 (98)	102 (11)	139 (11)	95 (2)	101 (5)	134 (9)
ω_3	205 (27)	155 (34)	145 (37)	113 (9)	119 (11)	137 (6)
ω_4	366 (133)	361 (39)	379 (29)	147 (21)	153 (42)	137 (47)
ω_5	791 (219)	769 (160)	791 (130)	614 (239)	534 (2)	336 (0)
ω_6	846 (297)	886 (154)	934 (109)	650 (215)	747 (165)	779 (126)
ω_7	1149 (54)	1138 (57)	1139 (44)	957 (1)	837 (127)	830 (104)
ω_8	3366 (2458)	3070 (183)	2698 (70)	1131 (103)	1135 (67)	1139 (53)
ω_9	3991 (246)	3237 (3334)	3059 (4384)	3676 (1495)	3301 (3350)	3098 (4232)

^a Infrared intensities (km mol^{-1}) are given in parentheses.

Table 5
MP2(full)/6-31++G(d,p) unscaled vibrational frequencies (cm^{-1}) of $\text{SiOH}^+-\text{XY}(\text{YX})$ complexes ($\text{X} = \text{Y} = \text{F}, \text{Cl}$ and Br) and SiOH^+ ion^a

Frequency	SiOHFCI^+	SiOHFBr^+	SiOHClBr^+	SiOHBrCl^+	SiOH^+
ω_1	49 (4)	33 (6)	33 (5)	43 (3)	583 (288)
ω_2	111 (4)	109 (13)	106 (6)	136 (44)	1078 (143)
ω_3	121 (12)	110 (4)	105 (9)	138 (6)	3707 (644)
ω_4	204 (56)	202 (58)	158 (51)	154 (10)	
ω_5	754 (70)	640 (125)	445 (3)	454 (0)	
ω_6	762 (227)	783 (214)	764 (149)	780 (136)	
ω_7	834 (197)	843 (189)	795 (109)	864 (106)	
ω_8	1143 (56)	1147 (41)	1138 (60)	1137 (55)	
ω_9	3375 (2856)	3277 (3557)	3234 (3658)	3131 (4168)	

^a Infrared intensities (km mol^{-1}) are given in parentheses.

Table 6
Complexation energies (E_{comp} in kcal/mol) and charge transfer Q_t (electron) from isolated XH , X_2 and XY to SiOH^+

Complexes	E_{comp}	Q_t
SiOHFH^+	-11.75	0.05
SiOHClH^+	-8.32	0.09
SiOHBrH^+	-10.85	0.13
SiOHF_2^+	-2.56	0.03
SiOHCl_2^+	-6.22	0.09
SiOHBr_2^+	-10.90	0.12
SiOHFCI^+	-9.00	0.05
SiOHFBr^+	-12.22	0.06
SiOHClBr^+	-8.31	0.10
SiOHBrCl^+	-9.38	0.12

Table 7
Energy (kcal/mol) of the proton transfer process calculated at QCISD(T)/6-31++G(d,p)//MP2(full)/6-31++G(d,p) level with ZPE corrections

Proton transfer process	E
$\text{SiOH}^+ + \text{FH} \rightarrow \text{FH}_2^+ + \text{SiO}$	76.68
$\text{SiOH}^+ + \text{ClH} \rightarrow \text{ClH}_2^+ + \text{SiO}$	56.32
$\text{SiOH}^+ + \text{BrH} \rightarrow \text{BrH}_2^+ + \text{SiO}$	50.61
$\text{SiOH}^+ + \text{F}_2 \rightarrow \text{F}_2\text{H}^+ + \text{SiO}$	113.26
$\text{SiOH}^+ + \text{Cl}_2 \rightarrow \text{Cl}_2\text{H}^+ + \text{SiO}$	60.80
$\text{SiOH}^+ + \text{Br}_2 \rightarrow \text{Br}_2\text{H}^+ + \text{SiO}$	50.27
$\text{SiOH}^+ + \text{FCI} \rightarrow \text{FCIH}^+ + \text{SiO}$	73.85
$\text{SiOH}^+ + \text{FCl} \rightarrow \text{ClFH}^+ + \text{SiO}$	75.06
$\text{SiOH}^+ + \text{FBr} \rightarrow \text{FBrH}^+ + \text{SiO}$	65.06
$\text{SiOH}^+ + \text{FBr} \rightarrow \text{BrFH}^+ + \text{SiO}$	64.17
$\text{SiOH}^+ + \text{ClBr} \rightarrow \text{ClBrH}^+ + \text{SiO}$	54.10
$\text{SiOH}^+ + \text{ClBr} \rightarrow \text{BrClH}^+ + \text{SiO}$	55.08

accompanied by a red-shift and intensity enhancement of the O–H stretch fundamental, $\Delta\nu_1$ and ΔI_1 . These observations are typical for hydrogen bonding and become more pronounced as the interaction strength increases: $\Delta r_{\text{O-H}} = 0.011, 0.016, 0.025 \text{ \AA}$; $\Delta\nu_1 = -341, -470, -640 \text{ cm}^{-1}$; $\Delta I_1 = 282, 418, 582\%$ and $E_{\text{comp}} = -11.75, -8.32, -10.85 \text{ kcal/mol}$ for $\text{X} = \text{F}, \text{Cl}, \text{Br}$, respectively. The same observations are reported on the SiOH^+-X ($\text{X} = \text{He}, \text{Ne}, \text{Ar}, \text{N}_2$) dimmers [26]. On the other hand, the calculated H^+-X bond lengths are 1.532, 2.102 and 2.200 \AA , respectively, for $\text{X} = \text{F}, \text{Cl}$ and Br . We noticed that the association of SiOH^+ with XH does not affect the Si–O and X–H distances significantly (Table 1): the Si–O distance becomes only slightly shorter from 1.136 to 1.132 \AA and the X–H distance becomes longer by 0.045, 0.031 and 0.028 \AA , respectively, for $\text{X} = \text{F}, \text{Cl}$ and Br . These observations are indicated that the SiOH^+-XH ($\text{X} = \text{F}, \text{Cl}$ and Br) complexes are of proton-bond complexes types. The dissociative proton transfer processes of $\text{SiOH}^+ + \text{XH}$ into XH_2^+ and SiO (Scheme 1) are highly endothermic by about 76, 56 and 51 kcal/mol for $\text{SiOH}^+ + \text{FH}$, $\text{SiOH}^+ + \text{ClH}$ and $\text{SiOH}^+ + \text{BrH}$ systems, respectively (Table 7). Indeed, the structures are more stable as weak complexes between SiOH^+ and XH rather than XH_2^+ and SiO . These tendencies are

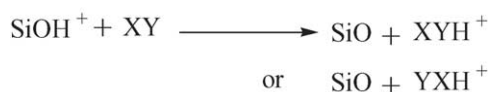


$\text{X} = \text{F}, \text{Cl}, \text{and Br}$

Scheme 1.

in good agreement with the O–H⁺ bond distance, which is more close to O–H⁺ distance in free SiOH⁺ fragment for SiOH⁺–XH complexes (Table 1). These results indicate that we cannot observe a direct dissociative proton transfer processes of SiOH⁺ + XH into XH₂⁺ and SiO. On the other hand, from the NBO results, we can see that the charge transfer from XH fragment to SiOH⁺ ion is more important in SiOH⁺–BrH complex than in SiOH⁺–ClH and SiOH⁺–FH ones (see Table 6).

In the SiOH⁺–X₂ (X=F, Cl and Br) dihalogen and SiOH⁺–XY(YX) (X=Y=F, Cl and Br) interhalogens complexes, the halogen atom also shares a proton with SiO and weakens the O–H⁺ bond strength. The O–H⁺ bond length becomes longer than in the isolated SiOH⁺ ion (Tables 2 and 3). In these complexes, we also observe a lengthening of the H⁺–O bond accompanied by a red-shift and intensity enhancement of the O–H stretch fundamental. On the other hand, we noticed that the association of SiOH⁺ with X₂ and XY does not affect the O–Si, X–X and X–Y distances significantly: the O–Si distance becomes slightly longer, the X–X distance becomes longer and the X–Y distance becomes shorter when the more polarisable atom is bonded and slightly longer when less polarisable atom is bonded. These observations indicated that the SiOH⁺–X₂, SiOH⁺–XY and SiOH⁺–YX complexes are of proton-bond complexes types. Indeed, the complexation energies are –2.56, –6.22 and –10.90 kcal/mol, respectively, for SiOH⁺–F₂, SiOH⁺–Cl₂ and SiOH⁺–Br₂. For the SiOH⁺–XY and SiOH⁺–YX complexes, the complexation energy are in range –8 to –12 kcal/mol. On the other hand, we noticed that the calculated H⁺–X bond lengths are longer in complex than in free protonated dihalogens X₂H⁺ and interhalogens YXH⁺, and XYH⁺. In addition, the dissociative proton transfer processes of SiOH⁺ + X₂ into X₂H⁺ and SiO (Scheme 2) are also endothermic by about 113, 61 and 50 kcal/mol for SiOH⁺ + F₂, SiOH⁺ + Cl₂ and SiOH⁺ + Br₂, respectively (Table 7). The dissociative proton transfer processes of SiOH⁺ + XY(YX) into XY(YX)H⁺ and SiO (Scheme 2) are also highly endothermic (Table 7). These results indicate that we cannot observe a direct dissociative proton transfer processes of SiOH⁺ + X₂ and SiOH⁺ + XY(YX) into X₂H⁺ and SiO, and XY(YX)H⁺ and SiO. On the other hand, from the NBO results, we can see that the intermolecular charge transfer from X₂, XH and XY fragments to SiOH⁺ ion is found more important in the bromine bonded complexes (Table 6).



Scheme 2.

4. Conclusion

Complexes of SiOH⁺ with XH, X₂ and XY (X=Y=F, Cl and Br) were found to have C_s symmetry with a halogen atom shares a proton with SiO. Formation of ions SiOH⁺–XH, SiOH⁺–X₂ and SiOH⁺–XY(YX) (X=F, Cl and Br) were calculated to be exothermic by 3–12 kcal/mol at the QCISD(T)/6-31++G(d,p)//MP2(full)/6-31++G(d,p)+ZPE level of theory. The calculated energetic results show that the stability of the ions depends on the type of the halogen bonded to SiOH⁺. The possible proton transfer dissociation processes of SiOH⁺ + XH, SiOH⁺ + X₂ and SiOH⁺ + XY complexes into XH₂⁺, X₂H⁺, XYH⁺ and YXH⁺, and SiO are calculated to be highly endothermic. The NBO results show that the largest intermolecular charge transfer is found in the Br bonded complexes. These observations are indicated that the SiOH⁺–XH, SiOH⁺–X₂, SiOH⁺–XY(YX) complexes should be experimentally observable in the gas phase.

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