

Electronic Supporting Information (ESI)

Table of Contents

Description of $\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{-Ar}$ isomers

Tables S1-S3. Computed vibrational frequencies (in cm^{-1} , B3LYP-D3/aug-cc-pVTZ) of: **(S1)** $\text{SiH}_3\text{OH}_2^+$ and $\text{SiH}_3\text{OH}_2^+\text{-Ar(I/II)}$, **(S2)** $\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{(I-IV)}$, and **(S3)** $\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{(I-IV)-Ar(I-IV)}$ compared to experimental values.

Tables S4-S9. Various energies (kJ mol^{-1}) calculated at the B3LYP-D3/cc-pVTZ level: **(S4)** $\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{(I-IV)}$; **(S5)** I-Ar(I-IV); **(S6)** II-Ar(I-IV); **(S7)** III-Ar(I-IV); **(S8)** IV-Ar(I-IV); **(S9)** (I-IV)-Ar(I-IV).

Figure S1. Typical mass spectrum of the ion source in the mass range m/z 10-130 for the pulsed supersonic plasma expansion of a $\text{SiH}_4/\text{He}/\text{Ar}$ gas mixture (ratio 1:20:200) at 5 bar stagnation pressure seeded with H_2O .

Figure S2. Collision-induced dissociation (CID) spectrum of size-selected $\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{-Ar}$ clusters to illustrate the loss of Ar and SiH_4 as major fragmentation channel and to verify the composition of the investigated mass-selected parent ions.

Figure S3. NBO charge distribution (in me) of SiH_4 , $\text{SiH}_3\text{OH}_2^+$, and $\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{(I-IV)}$ in their ground electronic state (B3LYP-D3/aug-cc-pVTZ).

Figures S4-S7. IRPD spectrum of $\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{-Ar}$ compared to linear IR absorption spectra of **(I-IV)-Ar(I-IV)** together with their equilibrium structures calculated at the B3LYP-D3/aug-cc-pVTZ level. Differences in relative energy (E_0) are given in kJ mol^{-1} . **(S4)** I-Ar(I-IV); **(S5)** II-Ar(I-IV); **(S6)** III-Ar(I-IV); **(S7)** IV-Ar(I-IV).

Figure S8. Visualization of molecular orbitals (MO) of $\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{(I)}$.

Cartesian coordinates (in Å) and energies (in hartree) of all relevant structures

Description of $\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{-Ar}$ isomers

$\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{-Ar(I-IV)}$ isomers are calculated for each $\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{(I-IV)}$ isomer, which are shown in Figures S4-S7 along with their spectra compared to the experimental $\text{SiH}_3\text{OH}_2^+\text{SiH}_4\text{-Ar}$ spectrum and the spectrum of their untagged $\text{SiH}_3\text{OH}_2^+\text{SiH}_4$ isomer. The vibrational assignment is listed in Table S3 and all relevant energies are listed in Tables S5-S9. In the respective most stable (I-IV)-Ar(I) structures, Ar is bound to the free OH group at distances of 2.228, 2.223, 2.226, and 2.287 Å, with binding energies of $D_0=13.99$, 13.79, 13.45 and 11.28 kJ mol^{-1} . This leads to slight elongations of the involved O-H bonds by 7, 8, 8, and 6 mÅ and contractions of the adjacent O-H bonds by 5, 5, 4, and 1 mÅ for I-Ar(I), II-Ar(I), III-Ar(I) and IV-Ar(I), respectively. As a result, the $\nu_{\text{OH}}^f/\nu_{\text{OH}}^s$ modes of (I-IV)-Ar(I) are redshifted to 3448, 3442, 3442, and 3482 cm^{-1} and the $\nu_{\text{OH}}^b/\nu_{\text{OH}}^a$ modes of (I-IV)-Ar(I) are blueshifted by 76, 74, 73, and 46 cm^{-1} to 2934, 2925, 2958, and 3633 cm^{-1} , respectively. In the case of (I-III)-Ar(I), Ar attachment leads to a weakening of the dihydrogen bridges, whose binding distances are increased by 16, 25, and 26 mÅ, respectively. In the (I/II)-Ar(II) isomers ($E_0=5.64$ and 5.85 kJ mol^{-1}), Ar is bound almost perpendicularly ($\phi_{\text{OHAr}}=96.5^\circ$, 101.1°) to the H atom of the H_2O moiety in the dihydrogen bridge with bond distances of 3.206 and 3.247 Å and binding energies of $D_0=8.34$ and 8.26 kJ mol^{-1} , respectively. As a result, the O-H bonds are slightly shortened by 1 and 2 mÅ, leading to small blueshifts of the corresponding ν_{OH}^b modes by 12 and 18 cm^{-1} to 2870 and 2869 cm^{-1} . A corresponding computational approach for a III-Ar(II) isomer, where Ar is also bonded almost perpendicularly to the H atom of the H_2O group in the DHB, leads to a rotation of the $\text{SiH}_3/\text{SiH}_4$ groups and converges to the II-Ar(II) isomer. In IV-Ar(II) ($E_0=5.61$ kJ mol^{-1}), Ar is bound to the other free OH group with a binding energy of $D_0=11.02$ kJ mol^{-1} , resulting in a similar elongation of the involved O-H bond by 1 mÅ and corresponding redshift of the ν_{OH}^s modes to 3482 cm^{-1} and blueshift of the ν_{OH}^a mode to 3634 cm^{-1} as for IV-Ar(I). In (I-III)-Ar(III) ($E_0=6.33$, 6.03, 5.56 kJ mol^{-1}), Ar is bound to the SiH_3 moiety with the same binding distance to Si of $R_{\text{SiAr}}=3.311$ Å and binding energies of $D_0=7.65$, 7.76, and 7.89 kJ mol^{-1} . As a result, the involved O-H bonds of the dihydrogen bridges are slightly shortened by 3 mÅ leading to blueshifts of the ν_{OH}^b modes by 43, 45, and 45 cm^{-1} to 2901, 2896, and 2930 cm^{-1} , respectively. In (IV)-Ar(III) ($E_0=7.30$ kJ mol^{-1}), Ar is bound almost perpendicularly ($\phi_{\text{SiHAr}}=91.5^\circ$) to the bridging H atom of the Si-H-Si bridge with a bond distance to H of $R_{\text{HAr}}=3.396$ Å and binding energies of $D_0=5.89$ kJ mol^{-1} . This affects the Si-H-Si bridge by shortening the Si-H and Si-H...Si bonds by 2 and 3 mÅ, respectively, but has almost no effect on the O-H bonds and their vibrational modes. In (I-III)-Ar(IV) ($E_0=10.09$, 9.88, 9.86 kJ mol^{-1}), Ar is bound to SiH_4 with binding distances to Si of $R_{\text{SiAr}}=3.617$, 3.617, and 3.627 Å and binding energies of $D_0=3.90$, 3.91, and 3.59 kJ mol^{-1} , respectively. This leads to a slight elongation of the O-H bonds involved in the dihydrogen bridge by 1, 2, and 2 mÅ, resulting in small redshifts of the corresponding ν_{OH}^b modes of 31, 29, and 28 cm^{-1} to 2827, 2822, and 2857 cm^{-1} , respectively. In (IV)-Ar(IV) ($E_0=7.30$ kJ mol^{-1}), Ar is also bound to SiH_4 with a bond distance to Si of $R_{\text{SiAr}}=3.563$ Å and a binding energy of $D_0=3.99$ kJ mol^{-1} . However, because SiH_4 is bound to the SiH_3 group here, Ar tagging has almost no effect on the O-H bonds and their vibrational modes.

Table S1. Computed vibrational frequencies (in cm^{-1} , B3LYP-D3/aug-cc-pVTZ) of $\text{SiH}_3\text{OH}_2^+$ and $\text{SiH}_3\text{OH}_2^+-\text{Ar}$ compared to experimental values. The experimental values are given with peak width (fwhm in parenthesis) and are assigned to the most dominant vibrations.^a

Mode	$\text{SiH}_3\text{OH}_2^+$	$\text{SiH}_3\text{OH}_2^+-\text{Ar}(\text{H})$	$\text{SiH}_3\text{OH}_2^+-\text{Ar}(\text{Si})$	Exp
$\nu_{\text{OH}}^{\text{b}(\text{Ar})}$		3369 (984)		C1 3400 (21)
$\nu_{\text{OH}}^{\text{s}}$	3550 (232)		3556 (237)	
$\nu_{\text{OH}}^{\text{f}}$		3602 (314)		E 3600 (30)
$\nu_{\text{OH}}^{\text{a}}$	3626 (319)		3632 (304)	

^aData taken from George et al., *Angew. Chem. Int. Ed.* 2018, **57**, 2919.

Table S2. Computed vibrational frequencies (in cm^{-1} , B3LYP-D3/aug-cc-pVTZ) of $\text{SiH}_3\text{OH}_2^+\text{SiH}_4(\text{I-IV})$ compared to experimental values of $\text{SiH}_3\text{OH}_2^+\text{SiH}_4$ (Figure 3). The experimental values are given with peak width (fwhm in parenthesis) and are assigned to the most dominant vibrations.

Mode	I	II	III	IV	Exp
$\nu_{\text{OH}}^{\text{b}(\text{SiH}_4)}$	2858 (2284)				A1 2830 (60)
$\nu_{\text{OH}}^{\text{b}(\text{SiH}_4)}$		2851 (2195)			
$\nu_{\text{OH}}^{\text{b}(\text{SiH}_4)}$			2885 (2011)		A2 2872 (50)
$2\beta_{\text{OH}}$	3212	3222	3216	3228	B 3194 (40)
$\nu_{\text{OH}}^{\text{s}}$				3587 (183)	D 3578 (20)
$\nu_{\text{OH}}^{\text{f}}$	3608 (233)				E 3602 (30)
$\nu_{\text{OH}}^{\text{f}}$		3605 (269)			
$\nu_{\text{OH}}^{\text{f}}$			3611 (287)		
$\nu_{\text{OH}}^{\text{a}}$				3662 (239)	F 3695 (10)

Table S3. Computed vibrational frequencies (in cm^{-1} , B3LYP-D3/aug-cc-pVTZ) of $\text{SiH}_3\text{OH}_2^+\text{SiH}_4(\text{I-IV})-\text{Ar}(\text{I-IV})$ compared to experimental values of $\text{SiH}_3\text{OH}_2^+\text{SiH}_4-\text{Ar}$ (Figure 4). The experimental values are given with peak width (fwhm in parenthesis) and are assigned to the most dominant vibrations.

Mode	$\nu_{\text{OH}}^{\text{b}(\text{SiH}_4)}$	$\nu_{\text{OH}}^{\text{b}(\text{SiH}_4)}$	$2\beta_{\text{OH}}$	$\nu_{\text{OH}}^{\text{b}(\text{Ar})}$	$\nu_{\text{OH}}^{\text{b}(\text{Ar})}$	$\nu_{\text{OH}}^{\text{s}}$	$\nu_{\text{OH}}^{\text{f}}$	$\nu_{\text{OH}}^{\text{a}}$
I-Ar(I)		2934 (2195)	3216	3448 (839)				
I-Ar(II)	2870 (2119)		3214				3615 (233)	
I-Ar(III)		2901 (2270)	3214				3611 (232)	
I-Ar(IV)	2827 (2413)		3210				3609 (226)	
II-Ar(I)		2925 (2125)	3216	3442 (921)				
II-Ar(II)	2869 (2034)		3222				3611 (276)	
II-Ar(III)		2896 (2162)	3222				3609 (270)	
II-Ar(IV)	2822 (2298)		3220				3605 (273)	
III-Ar(I)		2958 (1928)	3216	3442 (974)				
III-Ar(II)	n.a.		n.a.					n.a.
III-Ar(III)		2930 (1949)	3222				3614 (288)	
III-Ar(IV)	2857 (2085)		3218				3613 (293)	
IV-Ar(I)			3224	3482 (664)			3633 (283)	
IV-Ar(II)			3226	3482 (671)			3634 (279)	
IV-Ar(III)			3226			3579 (181)		3663 (235)
IV-Ar(IV)			3228			3580 (181)		3664 (234)
EXP	A1 2869 (20)	A2 2910 (70)	B 3232 (45)	C1 3456 (20)	C2 3495 (20)		E 3629 (15)	

Table S4. Various energies of the $\text{SiH}_3\text{OH}_2^+\text{SiH}_4(\text{I-IV})$ isomers calculated at the B3LYP-D3/aug-cc-pVTZ level. Energies are given in kJ mol^{-1} .

Isomer	E_0	E_e	G_0	$D_0(\text{SiH}_4)$
I	0.00	0.00	0.00	38.86
II	0.13	-0.12	1.56	38.73
III	0.40	-0.19	3.59	38.46
IV	2.64	1.37	4.14	36.23

Table S5. Various energies of the $\text{SiH}_3\text{OH}_2^+\text{SiH}_4(\text{I})\text{-Ar}(\text{I-IV})$ isomers calculated at the B3LYP-D3/aug-cc-pVTZ level. Energies are given in kJ mol^{-1} .

	E_0	E_e	G_0	$D_0(\text{Ar})$
I-Ar(I)	0.00	0.00	0.00	13.99
I-Ar(II)	5.64	5.91	12.18	8.34
I-Ar(III)	6.33	6.25	11.33	7.65
I-Ar(IV)	10.09	10.39	11.08	3.90

Table S6. Various energies of the $\text{SiH}_3\text{OH}_2^+\text{SiH}_4(\text{II})\text{-Ar}(\text{I-IV})$ isomers calculated at the B3LYP-D3/aug-cc-pVTZ level. Energies are given in kJ mol^{-1} .

	E_0	E_e	G_0	$D_0(\text{Ar})$
II-Ar(I)	0.00	0.00	0.00	13.79
II-Ar(II)	5.53	5.46	16.55	8.26
II-Ar(III)	6.03	6.16	11.65	7.76
II-Ar(IV)	9.88	10.30	13.41	3.91

Table S7. Various energies of the $\text{SiH}_3\text{OH}_2^+\text{SiH}_4(\text{III})\text{-Ar}(\text{I-IV})$ isomers calculated at the B3LYP-D3/aug-cc-pVTZ level. Energies are given in kJ mol^{-1} .

	E_0	E_e	G_0	$D_0(\text{Ar})$
III-Ar(I)	0.00	0.00	0.00	13.45
III-Ar(II)	n.a.	n.a.	n.a.	n.a.
III-Ar(III)	5.56	6.21	4.80	7.89
III-Ar(IV)	9.86	10.38	8.64	3.59

Table S8. Various energies of the $\text{SiH}_3\text{OH}_2^+\text{SiH}_4(\text{IV})\text{-Ar}(\text{I-IV})$ isomers calculated at the B3LYP-D3/aug-cc-pVTZ level. Energies are given in kJ mol^{-1} .

	E_0	E_e	G_0	$D_0(\text{Ar})$
IV-Ar(I)	0.00	0.00	0.00	11.28
IV-Ar(II)	0.27	0.03	1.68	11.02
IV-Ar(III)	5.39	5.82	9.13	5.89
IV-Ar(IV)	7.30	7.54	8.98	3.99

Table S9. Various energies of the $\text{SiH}_3\text{OH}_2^+\text{SiH}_4(\text{I-IV})\text{-Ar(I-IV)}$ isomers calculated at the B3LYP-D3/aug-cc-pVTZ level. Energies are given in kJ mol^{-1} .

	E_0^{tot}	E_e^{tot}	G_0^{tot}	$D_0(\text{Ar})$
I-Ar(I)	0.00	0.00	0.00	13.99
II-Ar(I)	0.33	-0.02	-0.41	13.79
III-Ar(I)	0.94	-0.29	8.83	13.45
IV-Ar(I)	5.34	3.70	9.55	11.28
IV-Ar(II)	5.61	3.74	11.23	11.02
I-Ar(II)	5.64	5.91	12.18	8.34
II-Ar(II)	5.85	5.45	16.14	8.26
III-Ar(II)	n.a.	n.a.	n.a.	n.a.
I-Ar(III)	6.33	6.25	11.33	7.65
II-Ar(III)	6.35	6.14	11.24	7.76
III-Ar(III)	6.50	5.93	13.63	7.89
I-Ar(IV)	10.09	10.39	11.08	3.90
II-Ar(IV)	10.21	10.29	13.00	3.91
IV-Ar(III)	10.73	9.52	18.69	5.89
III-Ar(IV)	10.80	10.09	17.47	3.59
IV-Ar(IV)	12.63	11.24	18.53	3.99

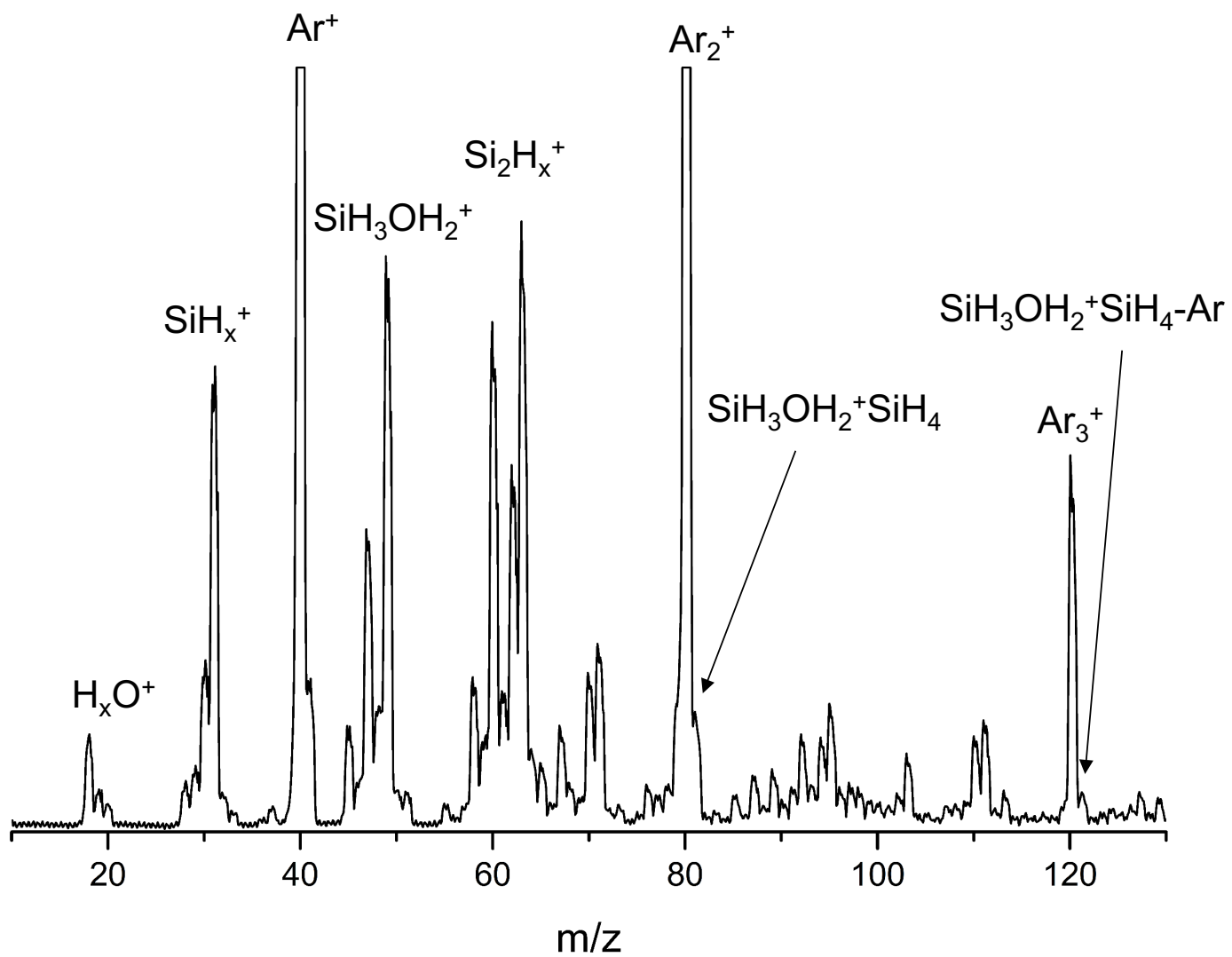


Figure S1

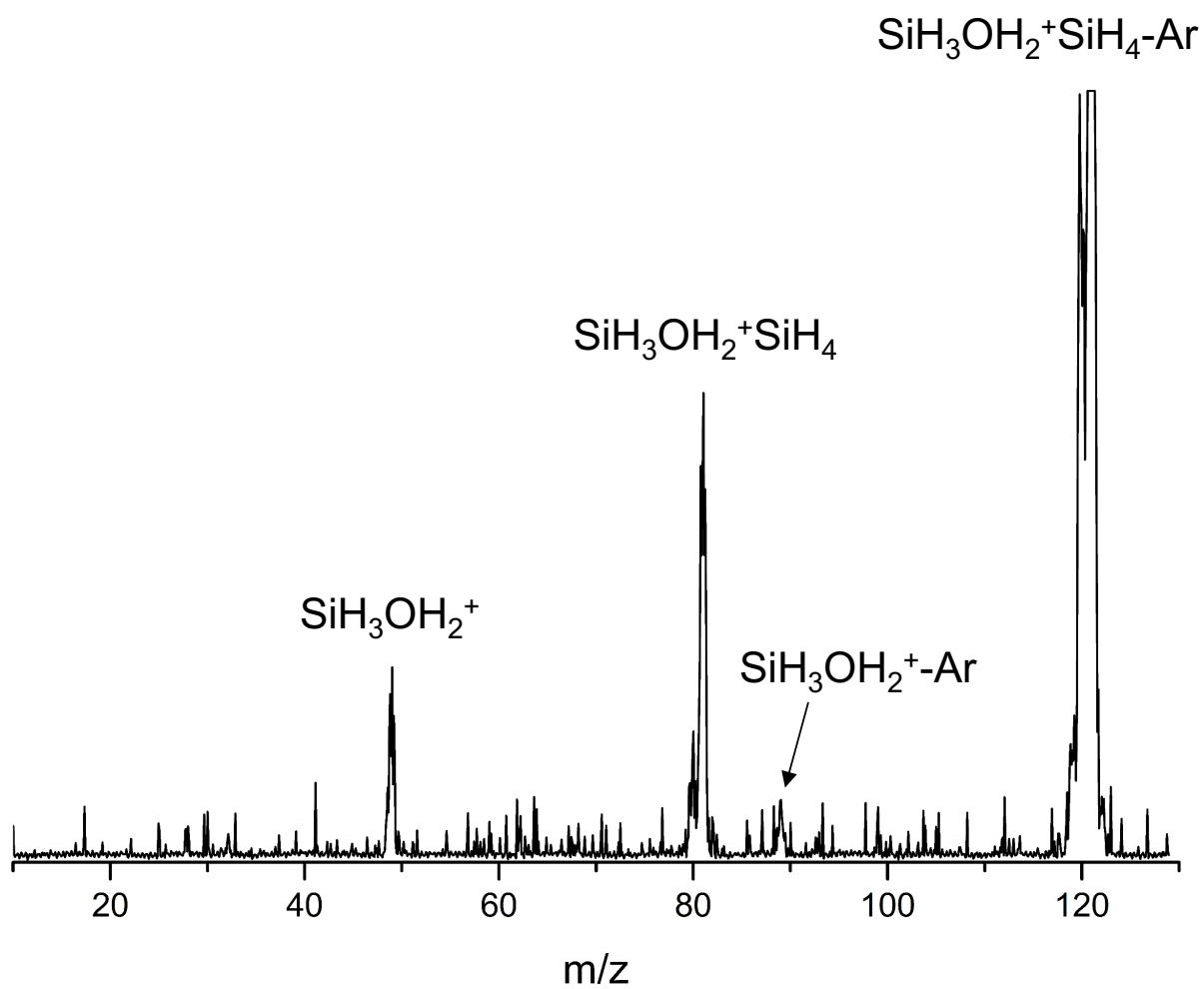


Figure S2

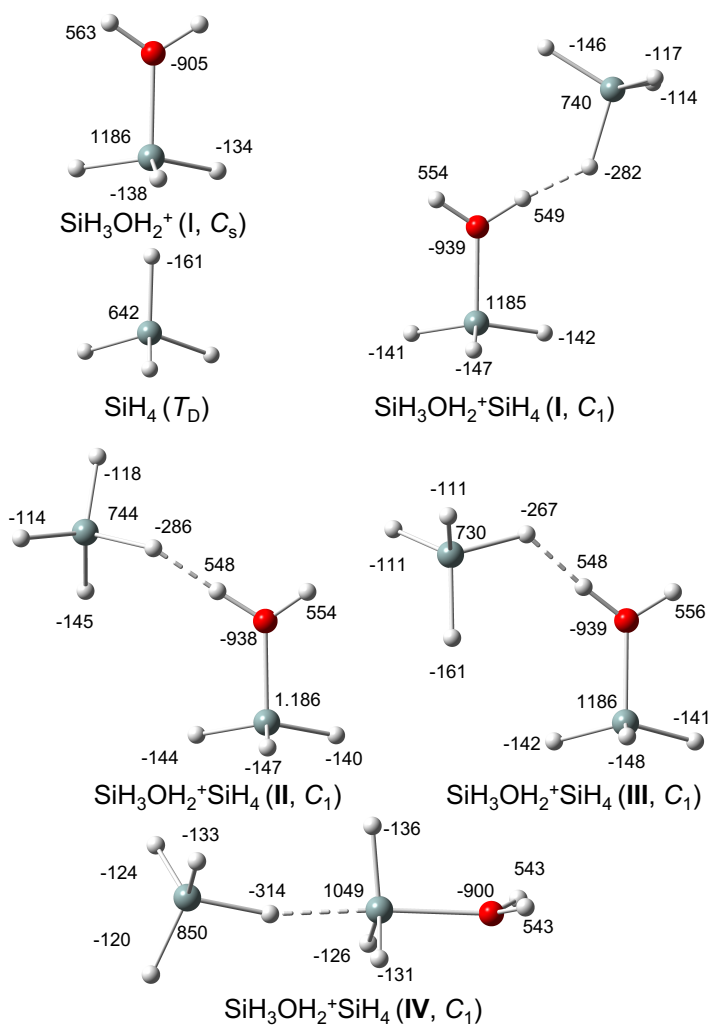


Figure S3

Figure S4

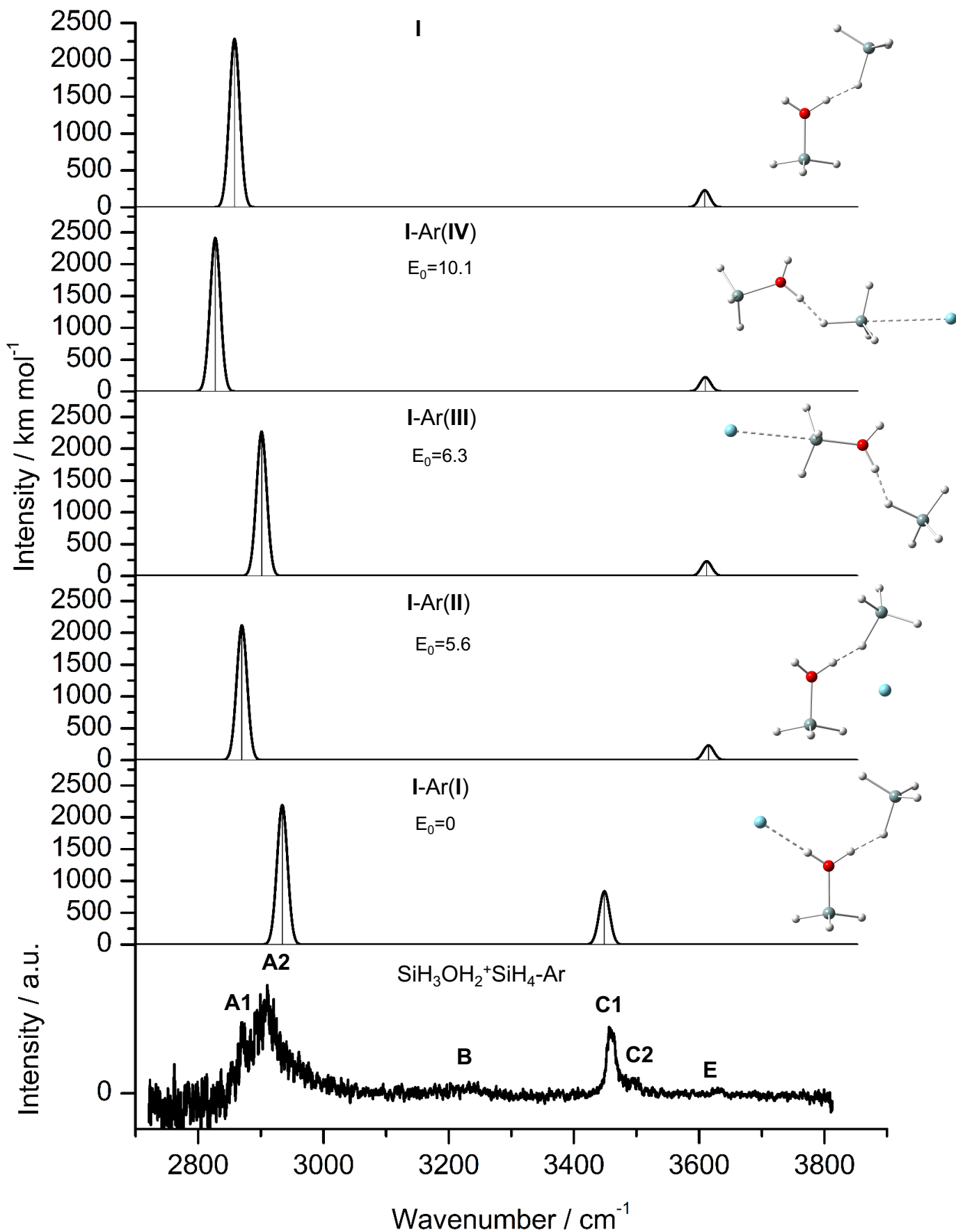


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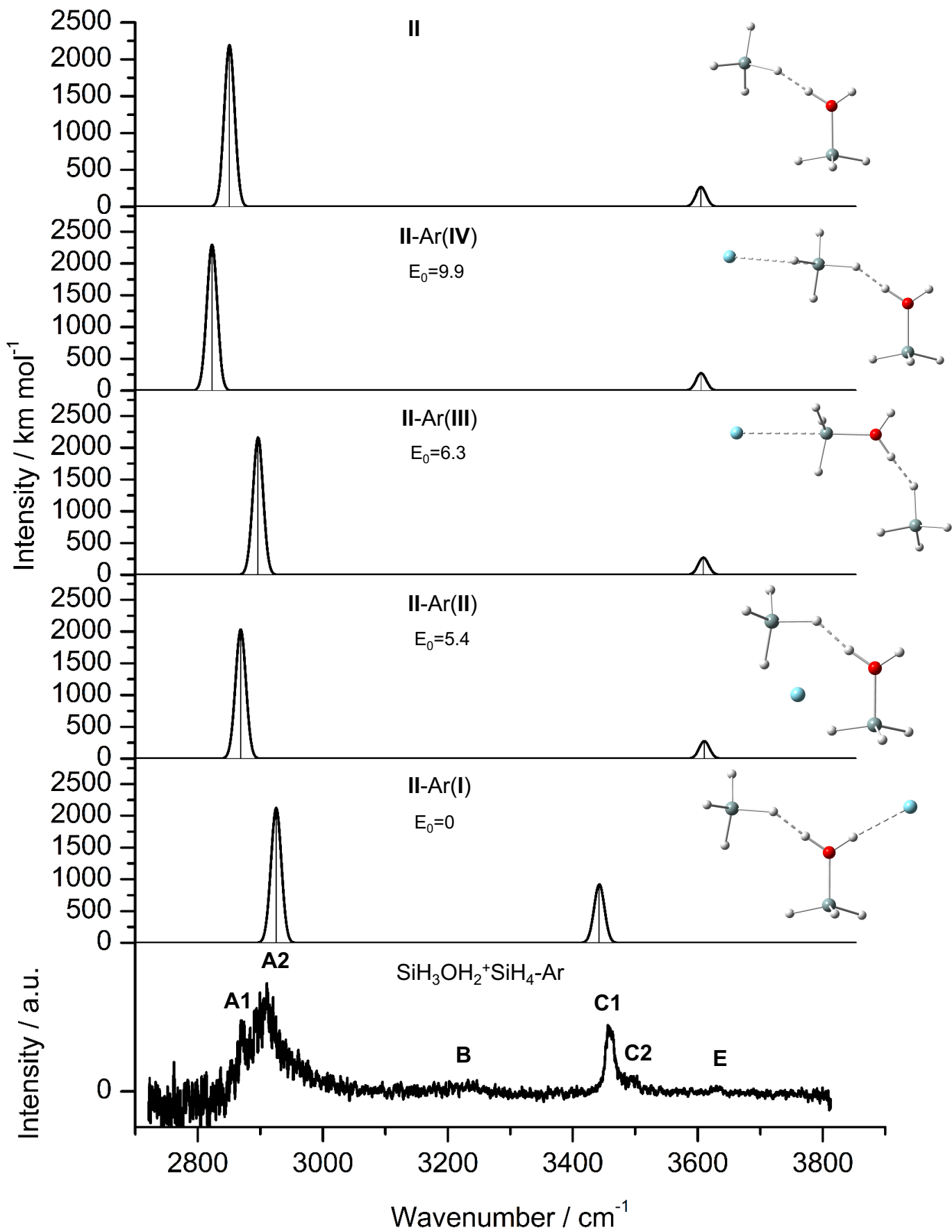


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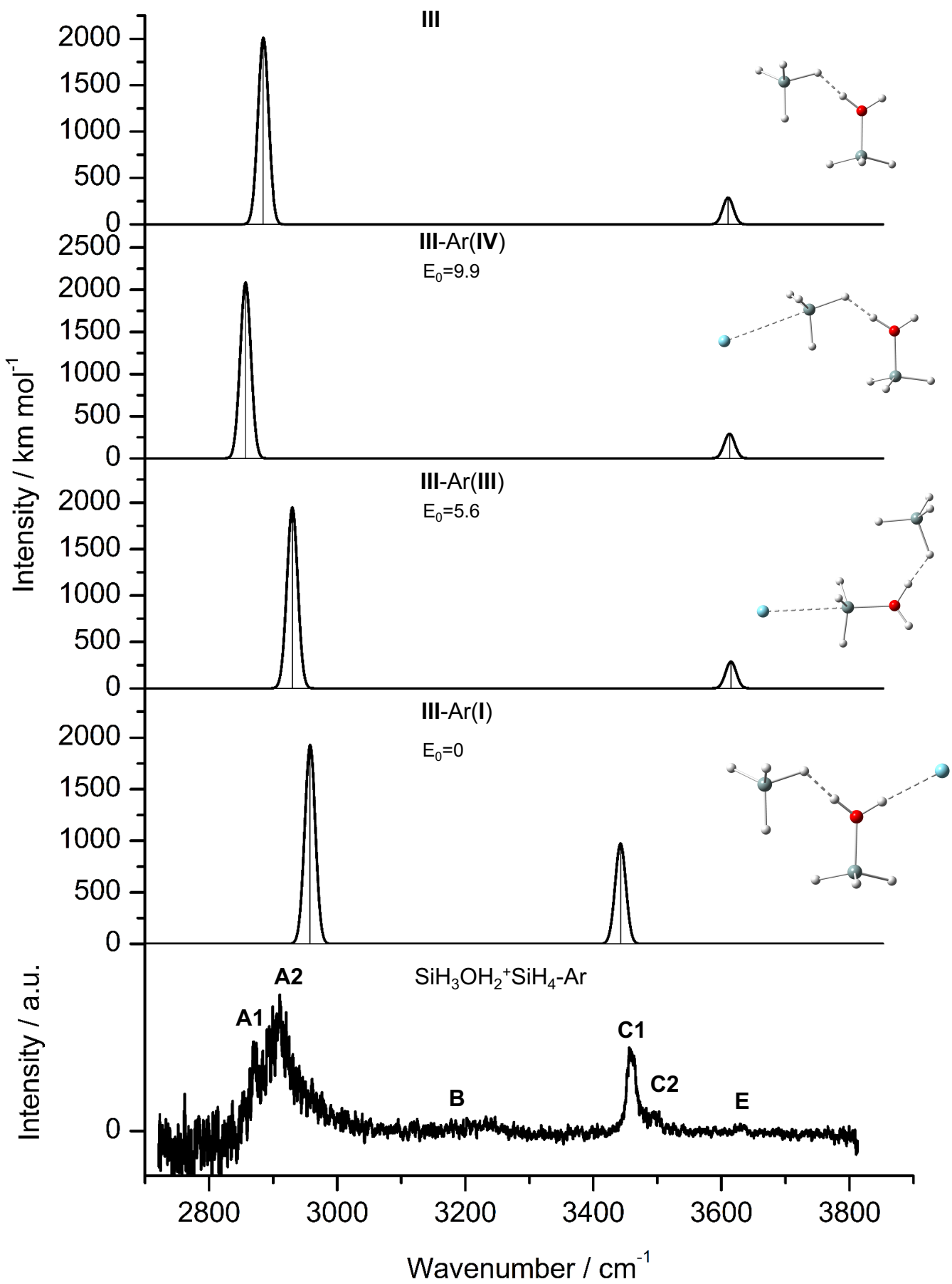


Figure S7

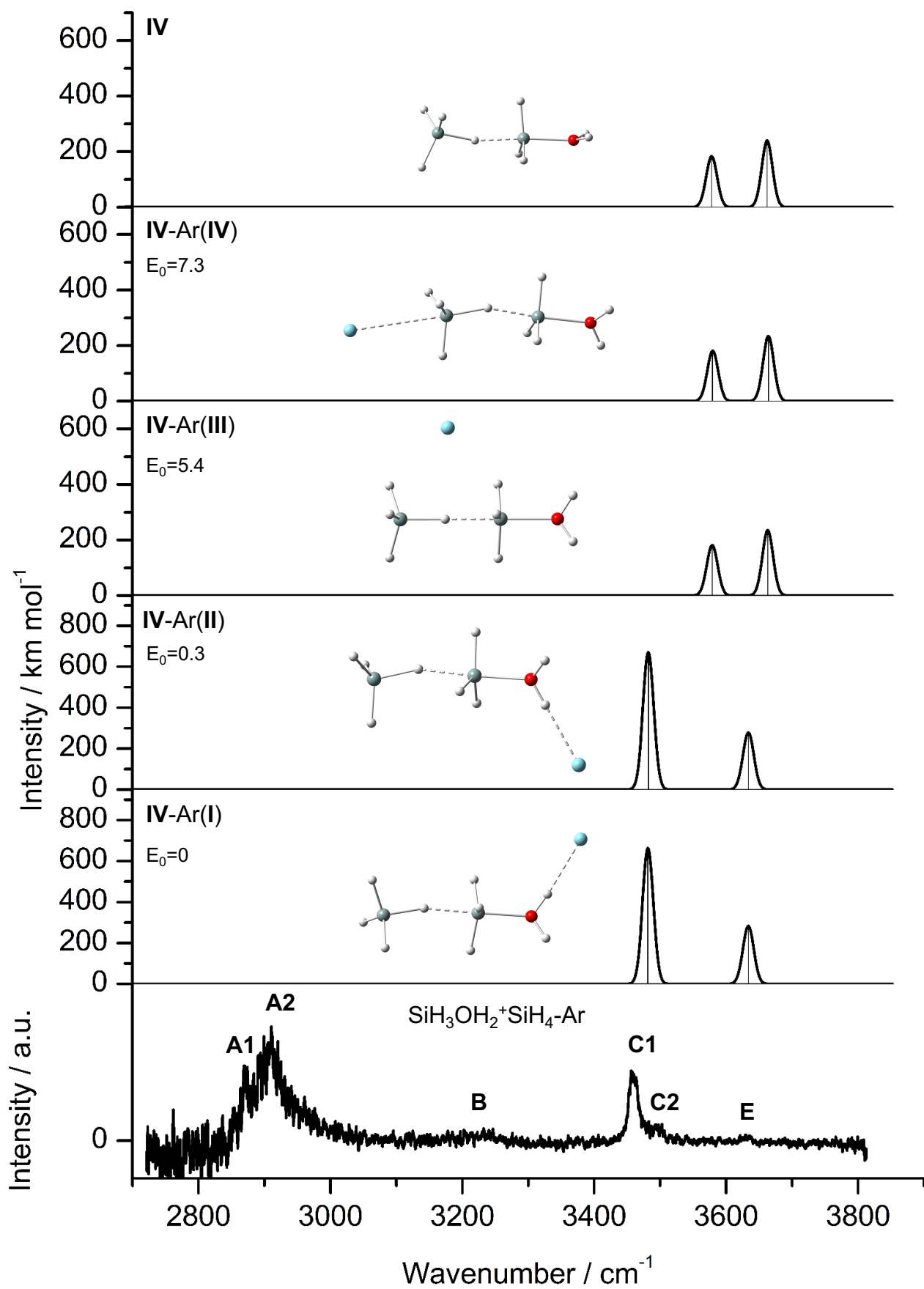
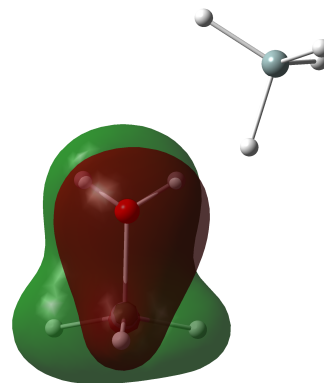
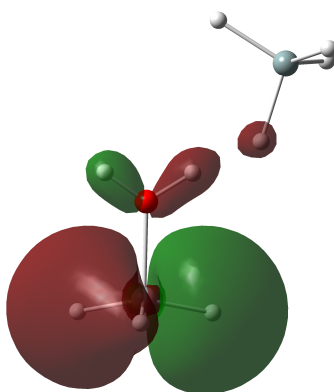
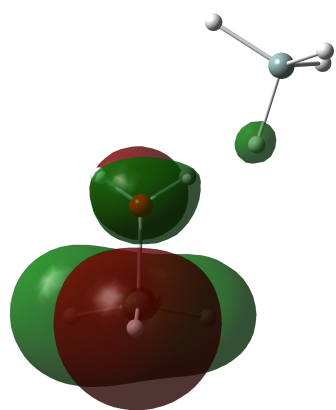
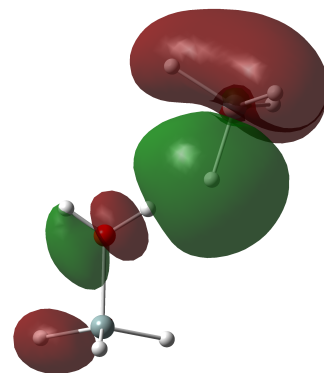
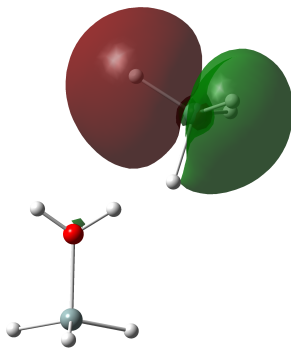
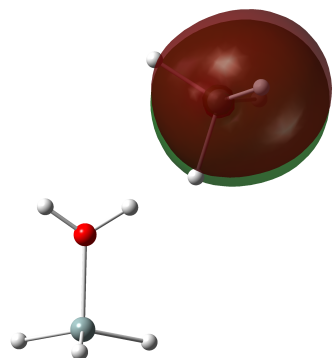


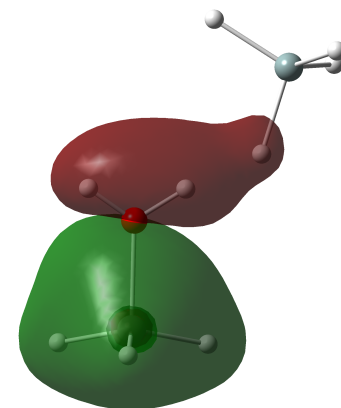
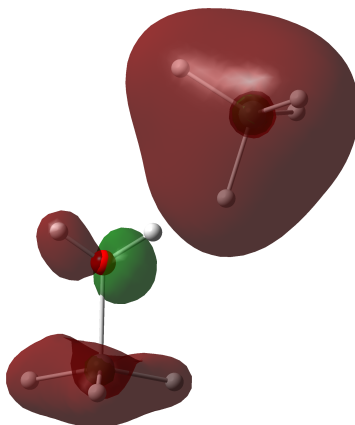
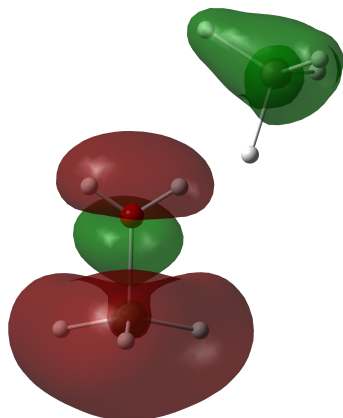
Figure S8



MO 19

MO 18

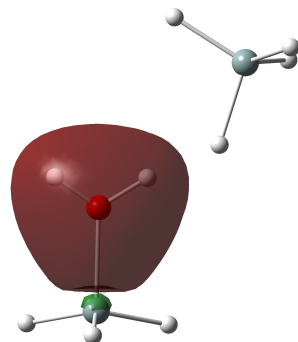
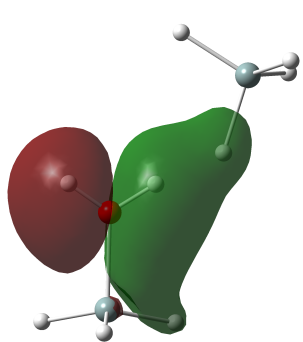
MO 17



MO 16

MO 15

MO 14



MO 13

MO 12

Cartesian coordinates (in Å) and energies (in hartree) of all relevant structures

Ar

Electronic energy= -527.560002

SiH₄

1	14	0	0.000000	0.000000	0.000000
2	1	0	0.856604	0.856604	0.856604
3	1	0	-0.856604	-0.856604	0.856604
4	1	0	-0.856604	0.856604	-0.856604
5	1	0	0.856604	-0.856604	-0.856604

Sum of electronic and zero-point Energies= -291.888507
 Sum of electronic and thermal Energies= -291.885447
 Sum of electronic and thermal Enthalpies= -291.884503
 Sum of electronic and thermal Free Energies= -291.907719

SiH₃OH₂⁺

1	14	0	0.010328	-0.695118	0.000000
2	1	0	0.733137	-0.928005	-1.254189
3	1	0	-1.416518	-1.035795	0.000000
4	1	0	0.733137	-0.928005	1.254189
5	8	0	0.010328	1.156158	0.000000
6	1	0	-0.138482	1.687099	-0.799132
7	1	0	-0.138482	1.687099	0.799132

Sum of electronic and zero-point Energies= -367.472638
 Sum of electronic and thermal Energies= -367.467928
 Sum of electronic and thermal Enthalpies= -367.466984
 Sum of electronic and thermal Free Energies= -367.498222

SiH₃OH₂⁺SiH₄(I)

1	14	0	-2.376994	-0.276955	0.003662
2	1	0	-3.241372	0.551669	-0.843685
3	1	0	-2.744533	-0.323739	1.424024
4	1	0	-1.905128	-1.540581	-0.572619
5	8	0	-0.828782	0.670833	-0.034528
6	1	0	-0.787322	1.623898	0.135889
7	1	0	0.079229	0.241899	0.063900
8	14	0	2.714461	-0.110385	-0.001686
9	1	0	3.138967	-0.840971	-1.208364
10	1	0	3.400961	-0.517020	1.236364
11	1	0	2.707743	1.355356	-0.197579
12	1	0	1.257163	-0.494414	0.210627

Sum of electronic and zero-point Energies= -659.375932
 Sum of electronic and thermal Energies= -659.367093
 Sum of electronic and thermal Enthalpies= -659.366149
 Sum of electronic and thermal Free Energies= -659.411831

SiH₃OH₂⁺SiH₄(II)

1	14	0	2.161284	-0.404064	-0.001122
2	1	0	2.651111	-0.430758	1.382425
3	1	0	3.120509	0.077511	-1.000936
4	1	0	1.311746	-1.533289	-0.394824
5	8	0	0.924166	0.923577	-0.021881
6	1	0	1.155071	1.860441	0.071271
7	1	0	-0.049950	0.768268	0.193008
8	14	0	-2.563248	-0.146421	-0.010148
9	1	0	-3.390605	0.866137	-0.688949
10	1	0	-3.204898	-0.781170	1.153948
11	1	0	-1.979052	-1.126705	-0.949387
12	1	0	-1.379753	0.617747	0.566268

Sum of electronic and zero-point Energies= -659.375883
 Sum of electronic and thermal Energies= -659.367141

Sum of electronic and thermal Enthalpies= -659.366196
 Sum of electronic and thermal Free Energies= -659.411236

SiH₃OH₂⁺SiH₄(III)

1	14	0	2.003314	-0.455886	0.003373
2	1	0	3.310474	0.171178	-0.222542
3	1	0	1.449109	-1.239761	-1.104939
4	1	0	1.791363	-1.021667	1.340935
5	8	0	0.937456	1.013411	-0.036823
6	1	0	1.258564	1.895729	0.202868
7	1	0	-0.069058	0.976561	-0.028497
8	14	0	-2.419601	-0.151687	0.003592
9	1	0	-3.189533	-0.102693	-1.250506
10	1	0	-3.216666	0.001563	1.232226
11	1	0	-1.520783	-1.328669	0.063150
12	1	0	-1.485097	1.046477	-0.035625

Sum of electronic and zero-point Energies= -659.375778
 Sum of electronic and thermal Energies= -659.367076
 Sum of electronic and thermal Enthalpies= -659.366132
 Sum of electronic and thermal Free Energies= -659.410464

SiH₃OH₂⁺SiH₄(IV)

1	14	0	0.893595	0.060105	-0.037657
2	1	0	0.921960	1.374991	-0.683796
3	1	0	0.682877	-0.014545	1.411212
4	1	0	0.764833	-1.163855	-0.832522
5	8	0	2.838112	-0.060021	-0.002396
6	1	0	3.401973	0.688495	0.241901
7	1	0	3.307864	-0.889188	0.169974
8	1	0	-2.537258	-1.325553	0.706490
9	14	0	-2.485362	-0.023854	0.016869
10	1	0	-3.050559	-0.041058	-1.343204
11	1	0	-2.922822	1.110549	0.848633
12	1	0	-0.989024	0.232824	-0.208488

Sum of electronic and zero-point Energies= -659.374928
 Sum of electronic and thermal Energies= -659.365826
 Sum of electronic and thermal Enthalpies= -659.364882
 Sum of electronic and thermal Free Energies= -659.410253

SiH₃OH₂⁺SiH₄(I)-Ar(I)

1	14	0	1.296506	2.239831	0.038317
2	1	0	2.476062	1.968292	-0.790904
3	1	0	1.557480	2.355191	1.478397
4	1	0	0.321741	3.193030	-0.503251
5	8	0	0.372611	0.699321	-0.140892
6	1	0	0.783462	-0.184885	-0.093279
7	1	0	-0.627412	0.646079	-0.069493
8	14	0	-3.160973	-0.304444	0.015900
9	1	0	-3.989646	0.043221	-1.151371
10	1	0	-3.843400	-0.152807	1.313006
11	1	0	-2.500130	-1.619573	-0.126171
12	1	0	-2.034946	0.713922	0.032700
13	18	0	1.721024	-2.202914	0.015470

Sum of electronic and zero-point Energies= -1186.941261
 Sum of electronic and thermal Energies= -1186.930066
 Sum of electronic and thermal Enthalpies= -1186.929122
 Sum of electronic and thermal Free Energies= -1186.985282

SiH₃OH₂⁺SiH₄(I)-Ar(II)

1	14	0	-2.419642	-0.580650	0.273942
2	1	0	-3.337428	-1.715876	0.128203
3	1	0	-2.795210	0.627539	-0.468538
4	1	0	-1.859898	-0.366038	1.612451
5	8	0	-0.929159	-1.164434	-0.576142
6	1	0	-0.884920	-1.348273	-1.526057
7	1	0	-0.010162	-1.122722	-0.163951
8	14	0	2.612214	-0.884592	0.123416
9	1	0	3.351050	-2.122061	0.427315
10	1	0	3.049952	0.294846	0.889350
11	1	0	2.526434	-0.615352	-1.328429
12	1	0	1.183432	-1.145919	0.569605
13	18	0	0.195223	2.074596	-0.060768
Sum of electronic and zero-point Energies=			-1186.939112		
Sum of electronic and thermal Energies=			-1186.927815		
Sum of electronic and thermal Enthalpies=			-1186.926871		
Sum of electronic and thermal Free Energies=			-1186.980642		

SiH₃OH₂⁺SiH₄(I)-Ar(III)

1	14	0	-0.804113	0.520499	0.017463
2	1	0	-1.449263	1.548570	-0.804413
3	1	0	-1.128689	0.550976	1.447578
4	1	0	-0.646790	-0.809641	-0.577431
5	8	0	0.931753	1.074921	-0.052272
6	1	0	1.200518	1.989250	0.122211
7	1	0	1.708382	0.443171	0.049184
8	14	0	4.188237	-0.551473	-0.001284
9	1	0	4.433110	-1.384183	-1.191738
10	1	0	4.751606	-1.090366	1.248567
11	1	0	4.541091	0.867952	-0.220097
12	1	0	2.681625	-0.567057	0.202286
13	18	0	-3.940186	-0.539689	-0.004693
Sum of electronic and zero-point Energies=			-1186.938849		
Sum of electronic and thermal Energies=			-1186.927545		
Sum of electronic and thermal Enthalpies=			-1186.926601		
Sum of electronic and thermal Free Energies=			-1186.980966		

SiH₃OH₂⁺SiH₄(I)-Ar(IV)

1	14	0	-4.176413	0.127006	0.019353
2	1	0	-4.970401	-0.860933	0.758078
3	1	0	-4.519324	0.275489	-1.400306
4	1	0	-3.848628	1.369713	0.726279
5	8	0	-2.542777	-0.661910	0.013842
6	1	0	-2.403267	-1.587171	-0.237888
7	1	0	-1.679856	-0.136876	-0.026247
8	14	0	0.901284	0.428562	-0.029257
9	1	0	1.376035	0.986853	1.247648
10	1	0	1.444787	1.081883	-1.231461
11	1	0	1.003806	-1.045515	-0.082147
12	1	0	-0.592776	0.724560	-0.063761
13	18	0	4.465758	-0.182815	0.018763
Sum of electronic and zero-point Energies=			-1186.937418		
Sum of electronic and thermal Energies=			-1186.926106		
Sum of electronic and thermal Enthalpies=			-1186.925162		
Sum of electronic and thermal Free Energies=			-1186.981062		

SiH₃OH₂⁺SiH₄(II)-Ar(I)

1	14	0	-0.224580	2.189787	0.022526
2	1	0	-0.529425	2.450325	1.434986
3	1	0	-1.301310	2.513023	-0.919973
4	1	0	1.138949	2.530095	-0.398427
5	8	0	-0.161299	0.390324	-0.115211
6	1	0	-0.963438	-0.165148	-0.069852
7	1	0	0.663055	-0.144064	0.094775
8	14	0	3.217926	-1.002122	0.005018
9	1	0	3.322319	-2.160716	-0.899328
10	1	0	3.995780	-1.129197	1.249710
11	1	0	3.460587	0.280355	-0.689626
12	1	0	1.765356	-0.956627	0.448114
13	18	0	-2.898240	-1.275998	0.015871
Sum of electronic and zero-point Energies=					-1186.941137
Sum of electronic and thermal Energies=					-1186.930031
Sum of electronic and thermal Enthalpies=					-1186.929086
Sum of electronic and thermal Free Energies=					-1186.985438

SiH₃OH₂⁺SiH₄(II)-Ar(II)

1	14	0	2.225094	0.549170	-0.427776
2	1	0	2.719089	-0.751808	0.035780
3	1	0	3.214793	1.632479	-0.423991
4	1	0	1.300417	0.515633	-1.565116
5	8	0	1.081391	1.084141	0.872698
6	1	0	1.358245	1.280841	1.780129
7	1	0	0.077505	1.017953	0.806436
8	14	0	-2.411352	1.009582	-0.176632
9	1	0	-3.080815	2.315659	-0.049258
10	1	0	-3.261262	-0.148707	0.147683
11	1	0	-1.712190	0.855212	-1.470124
12	1	0	-1.317256	1.006981	0.877104
13	18	0	-0.296779	-2.123328	0.074527
Sum of electronic and zero-point Energies=					-1186.939032
Sum of electronic and thermal Energies=					-1186.927954
Sum of electronic and thermal Enthalpies=					-1186.927010
Sum of electronic and thermal Free Energies=					-1186.979134

SiH₃OH₂⁺SiH₄(II)-Ar(III)

1	14	0	0.684723	0.737333	0.018331
2	1	0	1.131264	0.961133	1.397484
3	1	0	1.391366	1.501286	-1.013656
4	1	0	0.298731	-0.636483	-0.317030
5	8	0	-0.961719	1.516441	-0.042529
6	1	0	-1.095629	2.473347	0.031764
7	1	0	-1.811265	1.017461	0.163632
8	14	0	-3.761237	-0.822913	-0.009123
9	1	0	-4.887071	-0.293330	-0.798348
10	1	0	-4.159140	-1.575688	1.192999
11	1	0	-2.780186	-1.552611	-0.840333
12	1	0	-3.021170	0.396867	0.516418
13	18	0	3.649891	-0.734744	-0.006756
Sum of electronic and zero-point Energies=					-1186.938842
Sum of electronic and thermal Energies=					-1186.927605
Sum of electronic and thermal Enthalpies=					-1186.926661
Sum of electronic and thermal Free Energies=					-1186.981000

SiH₃OH₂⁺SiH₄(II)-Ar(IV)

1	14	0	3.576302	-0.809940	0.075459
2	1	0	4.118631	-0.623530	1.426830
3	1	0	4.574157	-0.923929	-0.993777
4	1	0	2.405639	-1.688559	-0.020294
5	8	0	2.801249	0.778431	-0.331260
6	1	0	3.314011	1.577722	-0.525699
7	1	0	1.852102	1.012292	-0.072149
8	14	0	-0.803616	0.833095	0.190367
9	1	0	-1.456042	1.586768	-0.893362
10	1	0	-1.404481	1.021311	1.521230
11	1	0	-0.591318	-0.589251	-0.149775
12	1	0	0.593411	1.428877	0.310254
13	18	0	-4.146316	-0.519629	-0.093041
Sum of electronic and zero-point Energies=			-1186.937374		
Sum of electronic and thermal Energies=			-1186.926154		
Sum of electronic and thermal Enthalpies=			-1186.925209		
Sum of electronic and thermal Free Energies=			-1186.980332		

SiH₃OH₂⁺SiH₄(III)-Ar(I)

1	14	0	0.019768	2.082282	0.054734
2	1	0	-1.352364	2.524963	-0.218608
3	1	0	1.035494	2.457147	-0.934435
4	1	0	0.447820	2.178479	1.455637
5	8	0	-0.154507	0.310002	-0.246975
6	1	0	-1.011624	-0.149690	-0.159177
7	1	0	0.612495	-0.335383	-0.231794
8	14	0	3.113765	-1.054825	0.035839
9	1	0	3.843400	-1.420299	-1.189930
10	1	0	3.462992	-1.848559	1.226198
11	1	0	3.172467	0.402202	0.304537
12	1	0	1.649688	-1.339339	-0.244216
13	18	0	-3.027432	-1.074107	0.038865
Sum of electronic and zero-point Energies=			-1186.940904		
Sum of electronic and thermal Energies=			-1186.930027		
Sum of electronic and thermal Enthalpies=			-1186.929083		
Sum of electronic and thermal Free Energies=			-1186.981919		

SiH₃OH₂⁺SiH₄(III)-Ar(III)

1	14	0	-0.582102	0.773569	-0.004367
2	1	0	-1.473257	1.929779	0.134803
3	1	0	-0.454461	-0.111076	1.156553
4	1	0	-0.584073	0.111078	-1.312763
5	8	0	1.025903	1.632514	0.039851
6	1	0	1.124350	2.562957	-0.211169
7	1	0	1.911501	1.158639	0.033067
8	14	0	3.500971	-0.915622	-0.003705
9	1	0	4.221077	-1.227259	1.242306
10	1	0	4.265233	-1.152679	-1.240066
11	1	0	2.161881	-1.550371	-0.047907
12	1	0	3.221584	0.576378	0.035324
13	18	0	-3.525846	-0.742712	0.000225
Sum of electronic and zero-point Energies=			-1186.938786		
Sum of electronic and thermal Energies=			-1186.927588		
Sum of electronic and thermal Enthalpies=			-1186.926643		
Sum of electronic and thermal Free Energies=			-1186.980090		

SiH₃OH₂⁺SiH₄(III)-Ar(IV)

1	14	0	3.159448	-0.992063	-0.005322
2	1	0	4.618638	-0.972471	-0.159576
3	1	0	2.383120	-1.437791	-1.166588
4	1	0	2.663332	-1.453878	1.296435
5	8	0	2.820072	0.790053	-0.007289
6	1	0	3.485862	1.446621	0.246392
7	1	0	1.892888	1.187737	-0.007568
8	14	0	-0.696375	1.120269	-0.011858
9	1	0	-1.362427	1.503458	-1.266980
10	1	0	-1.374884	1.556552	1.219186
11	1	0	-0.344825	-0.318903	0.021442
12	1	0	0.643962	1.840578	-0.019788
13	18	0	-3.869403	-0.637067	0.007549
Sum of electronic and zero-point Energies=			-1186.937149		
Sum of electronic and thermal Energies=			-1186.926080		
Sum of electronic and thermal Enthalpies=			-1186.925136		
Sum of electronic and thermal Free Energies=			-1186.978627		

SiH₃OH₂⁺SiH₄(IV)-Ar(I)

1	14	0	0.605800	0.542147	-0.035207
2	1	0	0.235701	-0.509147	-0.986330
3	1	0	0.695873	0.204406	1.388635
4	1	0	1.241311	1.776947	-0.501880
5	8	0	-1.157481	1.304666	-0.018806
6	1	0	-1.958026	0.750046	0.008618
7	1	0	-1.346763	2.174454	0.361769
8	1	0	4.305686	0.456796	0.996466
9	14	0	3.853284	-0.548307	0.017131
10	1	0	4.446228	-0.381152	-1.321346
11	1	0	3.889042	-1.930487	0.526766
12	1	0	2.365849	-0.255165	-0.185239
13	18	0	-3.724568	-0.702099	0.006448
Sum of electronic and zero-point Energies=			-1186.939228		
Sum of electronic and thermal Energies=			-1186.927915		
Sum of electronic and thermal Enthalpies=			-1186.926970		
Sum of electronic and thermal Free Energies=			-1186.981643		

SiH₃OH₂⁺SiH₄(IV)-Ar(II)

1	14	0	-0.650853	0.715506	-0.023311
2	1	0	-1.177762	2.025910	-0.413568
3	1	0	-0.731653	0.314862	1.384724
4	1	0	-0.409208	-0.319737	-1.031194
5	8	0	1.175703	1.311996	-0.027423
6	1	0	1.446259	2.159062	0.355316
7	1	0	1.924725	0.689104	-0.012595
8	1	0	-3.296802	-1.999429	0.371232
9	14	0	-3.780244	-0.653415	0.012105
10	1	0	-4.424491	-0.587216	-1.311310
11	1	0	-4.537139	0.008846	1.089075
12	1	0	-2.512978	0.189630	-0.140045
13	18	0	3.686044	-0.769237	0.004702
Sum of electronic and zero-point Energies=			-1186.939126		
Sum of electronic and thermal Energies=			-1186.927867		
Sum of electronic and thermal Enthalpies=			-1186.926923		
Sum of electronic and thermal Free Energies=			-1186.981004		

SiH₃OH₂⁺SiH₄(IV)-Ar(III)

1	14	0	1.449089	-0.419081	0.008468
2	1	0	1.062074	0.244229	-1.238444
3	1	0	1.049227	0.178407	1.285376
4	1	0	1.950053	-1.796187	-0.002797
5	8	0	3.250313	0.325735	-0.049819
6	1	0	3.420753	1.257508	-0.251142
7	1	0	3.975450	-0.026787	0.486561
8	1	0	-2.295256	-1.280776	1.235841
9	14	0	-1.693162	-1.789626	-0.008342
10	1	0	-1.464602	-3.245217	-0.015617
11	1	0	-2.318503	-1.271044	-1.236928
12	1	0	-0.283520	-1.186432	-0.020186
13	18	0	-1.537842	1.969018	0.008563
Sum of electronic and zero-point Energies=					-1186.937174
Sum of electronic and thermal Energies=					-1186.925703
Sum of electronic and thermal Enthalpies=					-1186.924759
Sum of electronic and thermal Free Energies=					-1186.978164

SiH₃OH₂⁺SiH₄(IV)-Ar(IV)

1	14	0	2.604398	0.063687	-0.000823
2	1	0	2.774786	1.491616	-0.283055
3	1	0	2.369977	-0.367325	1.380773
4	1	0	2.387772	-0.896392	-1.086086
5	8	0	4.536201	-0.241086	-0.009346
6	1	0	5.158967	0.370108	0.410479
7	1	0	4.925213	-1.127339	-0.039428
8	1	0	-0.911218	-1.206783	0.181433
9	14	0	-0.753570	0.240997	-0.041616
10	1	0	-1.212907	0.703673	-1.361457
11	1	0	-1.183331	1.076765	1.091677
12	1	0	0.769287	0.452157	-0.093441
13	18	0	-4.293319	-0.157409	0.026000
Sum of electronic and zero-point Energies=					-1186.936449
Sum of electronic and thermal Energies=					-1186.924967
Sum of electronic and thermal Enthalpies=					-1186.924023
Sum of electronic and thermal Free Energies=					-1186.978224