

Supporting Information

Dipole-Bound Anions of Intramolecular Complexes

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Methods

Experimental

Anion photoelectron spectroscopy is conducted by crossing a mass-selected beam of negative ions with a fixed-frequency photon beam and energy-analyzing the resultant photodetached electrons. This technique is governed by the energy-conserving relationship, $h\nu = EKE + EBE$, where $h\nu$, EKE , and EBE are the photon energy, the electron kinetic energy, and the electron binding (transition) energy, respectively. Electron kinetic energies were measured using a velocity-map imaging (VMI) spectrometer.¹ Mass-selected anions were crossed with 1064 nm, linearly polarized photons in an electric field. The resultant photodetached electrons are accelerated along the axis of the ion beam toward a position-sensitive detector coupled to a CCD camera. The two-dimensional image formed from the sum of the electrons is reconstructed into a portion of the three-dimensional distribution via the BASEX² method. Photoelectron spectra are calibrated against the well-known spectrum of NO^- .³

In this work, silatrane anions were generated by a Rydberg electron transfer (RET) source. The neutral silatrane molecules, **HS** and **FS**, were vaporized in a heated pulsed valve then expanded with 10 psig of helium gas. The anions were formed when the neutral molecules collided with a thermally-expanded beam of potassium atoms, which had been excited to nd Rydberg states in two steps using two dye lasers. One dye laser pumped the potassium atoms to the $^2\text{P}_{3/2}$ state with 766.7 nm light, while the other was tuned to reach specific Rydberg levels. To get the most intense ion signals, the potassium atoms were pumped to the 14d Rydberg state for **HS**⁻ and 13d Rydberg state for **FS**⁻. The anions were then extracted using a time-of-flight mass

spectrometer and mass-selected, and their electrons were photodetached and energy-analyzed with velocity-map imaging spectroscopy.

Computational

All calculations were carried out using the Gaussian 09 program package.⁴ The geometries of the neutral molecules, **HS** and **FS**, were optimized in the restricted variants of the MP2 (6-311++G(d,p),⁵ aug-cc-pVDZ,⁶ and B2(s) basis sets) and the coupled-cluster singles and doubles (CCSD)⁷ (6-31++G(d,p) basis set) methods. The B2(s) basis set is a modification of the B2 basis set,⁸ including only s diffuse functions added on hydrogen atoms. The B2 basis is constructed by augmenting the 6-311++G(d,p)⁵ basis with a set of diffuse s and p functions. The exponents of these additional basis functions are obtained by dividing the smallest respective exponent of the 6-311++G(d,p) basis by a factor of three for oxygen, nitrogen, carbon, fluorine, and silicon atoms and are taken to be equal to 0.001 for each hydrogen atom.⁸ The unrestricted variants of these methods were applied for geometry optimizations of the dipole-bound anions, **HS⁻** and **FS⁻**, more specifically, the radical-anions, **HS^{-•}** and **FS^{-•}**. The geometry optimization did not converge for **HS⁻** and **FS⁻** when using the B2 basis set. The correspondence of the MP2 and UMP2, using the 6-311++G(d,p) and B2(s) basis sets, optimized structures to the minima on the potential energy surface was confirmed by the positive eigenvalues of the corresponding Hessians.

The vertical electron detachment energy (VDE), which was directly measured by negative ion photoelectron spectroscopy, is defined as the energy difference between the neutral molecule **HS(FS)** and its anion **HS⁻(FS⁻)** both at the equilibrium geometry of the anion. Based on the works of Skurski et al.,⁹ the VDE values were obtained from single-point calculations at the MP2 level with the aug-cc-pVDZ basis set supplemented with even-tempered⁹ diffuse functions centered on the positive end of the molecular dipole of **HS(FS)**. For example, on the N(CH₂)₃ fragment: 5s5p4d(N) and 7s7p8d(N) are the sets of 5s5p4d and 7s7p8d diffuse functions centered only on the nitrogen atom; 5s5p(H₃) are the functions on the three terminal hydrogen atoms; 5s5p4d(H₃N) corresponds the functions on the nitrogen atom and three hydrogen atoms. The values of exponents in 5s5p4d and 7s7p8d sets were calculated according to Skurski et al.⁹ The geometric progression ratio was equal to 3.2.⁹ For each symmetry, we started to build up the exponents of the extra diffuse functions from the lowest exponent of the same symmetry included in the aug-cc-pVDZ basis set for nitrogen and hydrogen. For the 5s5p4d set on the nitrogen atom, we achieved lowest exponents of 1.825×10^{-4} , 1.672×10^{-4} , and

2.193×10^{-3} a.u. for the s, p, and d symmetries, respectively. For the 7s7p8d set, they turned out to be equal to 1.782×10^{-5} , 1.633×10^{-5} , and 2.092×10^{-5} a.u., respectively. For the 5s5p set on the hydrogen atoms, the lowest exponents were 8.863×10^{-5} and 4.202×10^{-4} a.u. for s and p symmetry, respectively.

The VDE estimations were also performed using the MP2, CCSD and coupled-cluster singles and doubles with perturbative triples, CCSD(T), single-point calculations with the B2(s) and B2 basis sets. The adiabatic electron affinity (AEA) was calculated as the CCSD/B2 as well as the CCSD(T)/B2 energy difference between the neutral species and its anion at their own equilibrium geometries. Therewith the corresponding contributions from the MP2/B2(s) zero-point vibrational energies (ZPE) were taken into account. The problem of spin contamination for the UMP2 wave functions has not arisen for the anions, **HS⁻** and **FS⁻**. In all cases, the $\langle S^2 \rangle$ value turned out to be 0.750. Simulated photoelectron spectra of the dipole-bound anions, **HS⁻** and **FS⁻**, were generated using the Franck–Condon method¹⁰ as implemented¹¹ in Gaussian09 using the default parameters which include a convolution of the MP2/B2(s) spectra with Gaussian distribution functions with a FWHM of 270 cm^{-1} . Three-dimensional plots of the orbital amplitudes were generated using the MOLDEN program.¹²

The pentacoordinate character, or trigonal bipyramidal structure, of the silicon atom, η_e , was determined by Equation (1):¹³

$$\eta_e = \left[1 - \frac{120 - 1/3 \sum_{n=1}^3 \theta_n}{120 - 109.5} \right] \times 100\% \quad (1)$$

Here, θ_n refer to the bond angles between the equatorial bonds at the silicon atom. The Method2//Method1 notation implies that the calculation of properties (energy, normal vibrational modes, wave functions) was performed with the Method2 for a structure optimized with Method1.

Table S1. The dipole moments of the neutral silatranes $\text{XSi}(\text{OCH}_2\text{CH}_2)_3\text{N}$ calculated from the HF and MP2 densities with the B2(s) basis set ^a

	Neutral geometry	Anionic geometry	Neutral geometry	Anionic geometry
	X = H	X = H	X = F	X = F
$\mu^{\text{HF}}, \text{D}$	6.69	7.05	8.96	9.34
$\mu^{\text{MP2}}, \text{D}$	6.27	6.61	8.32	8.67

^a The geometries were optimized at the MP2/B2(s) level of theory.

Table S2. Selected experimental and calculated structural parameters of the molecules of silatranes $\text{XSi}(\text{OCH}_2\text{CH}_2)_3\text{N}$ and their dipole-bound anions (in bold).

X	Method	Basis set	d_{SiN} , Å	d_{XSi} , Å	d_{CO} , Å	$\angle\text{OSiO}$, deg	$\angle\text{NCC}$, deg	η_e , Å
H	(ED) ^a		2.406(27)	-	1.399(11)	116.3(13)	108.2(30)	65
	CCSD	6-31++G(d,p)	2.417	1.464	1.417	116.1	106.9	63
			2.182	1.474	1.418	118.4	106.1	85
	CCSD	6-311++G(d,p)	2.448	1.465	1.410	115.7	107.0	60
			2.207	1.475	1.411	118.2	106.1	83
	MP2	6-31++G(d,p)	2.327	1.465	1.417	117.0	106.5	72
			2.159	1.474	1.421	118.6	106.0	87
	MP2	6-311++G(d,p)	2.352	1.466	1.410	116.8	106.5	70
			2.175	1.475	1.413	118.5	105.8	86
	MP2	B2(s)	2.352	1.466	1.410	116.8	106.5	70
			2.300	1.468	1.411	117.4	106.2	75
	MP2	aug-cc-pVDZ	2.238	1.484	1.419	118.1	106.2	82
2.138			1.493	1.424	118.9	105.9	89	
MP2	aug-cc-pVTZ	2.268	1.471	1.407	117.6	106.2	77	
F	(ED) ^b		2.324(14)	1.568(6)	1.392(4)	117.8(1)	104.5(6)	79
	CCSD	6-31++G(d,p)	2.293	1.622	1.415	117.7	106.4	78
			2.135	1.640	1.418	119.0	105.8	90
	CCSD	6-311++G(d,p)	2.325	1.609	1.408	117.4	106.4	75
			2.153	1.628	1.411	118.8	105.7	89
	MP2	6-31++G(d,p)	2.252	1.628	1.417	118.0	106.1	81
			2.123	1.646	1.421	119.1	105.6	91
	MP2	6-311++G(d,p)	2.273	1.616	1.409	117.8	106.1	80
			2.139	1.634	1.413	119.0	105.6	90
	MP2	B2(s)	2.273	1.616	1.409	117.8	106.1	80
			2.223	1.622	1.411	118.3	105.8	84
	MP2	aug-cc-pVDZ	2.185	1.647	1.419	118.8	105.9	88
2.106			1.663	1.424	119.3	105.6	94	

^a Data of I. F. Shishkov, L. V. Khristenko, F. M. Rudakov, A. V. Golubinskii, L. V. Vilkov, S. S. Karlov, G. S. Zaitseva, S. Samdal, *Struct. Chem.* **2004**, *15*, 11-16. ^b Data of G. Forgacs, M. Kolonits, I. Hargittai, *Struct. Chem.* **1990**, *1*, 245.

Table S3. MP2/B2(s) values of Franck-Condon factors (FC factors), intensities (I), absolute (E) and relative (ΔE) transition energies in the photoelectron spectra of the anions of silatranes.^a

X	Transition	ΔE , cm ⁻¹	E , eV	FC factors	I	Assignment
H	0 ₀ ⁰	0	0.039	1.000	1.000	
	1 ₀ ¹	85	0.050	0.136	0.194	HSiO ₃ -N(CH ₂) ₃ twisting and Si-N stretching
	1 ₀ ²	171	0.060	0.008	0.015	O-Si-O bending
	4 ₀ ¹	235	0.068	0.031	0.067	Si-N stretching
	13 ₀ ¹	586	0.112	0.003	0.013	H-Si-O bending
	33 ₀ ¹	1182	0.185	0.001	0.006	C-O stretching
F	0	0	0.090	1.000	1.000	
	1 ₀ ¹	91	0.101	0.138	0.161	HSiO ₃ -N(CH ₂) ₃ twisting and Si-N stretching
	1 ₀ ²	181	0.112	0.009	0.012	O-Si-O bending
	6 ₀ ¹	237	0.119	0.043	0.061	Si-N stretching
	22 ₀ ¹	875	0.199	0.005	0.013	Si-F stretching

^a The FC factor and intensity for the 0–0 transitions were normalized to one and all other factors and intensities were scaled accordingly. The notation n_k^l means that for the n th mode there is an excitation from k to l quanta and 0₀⁰ stands for the 0–0 transition.

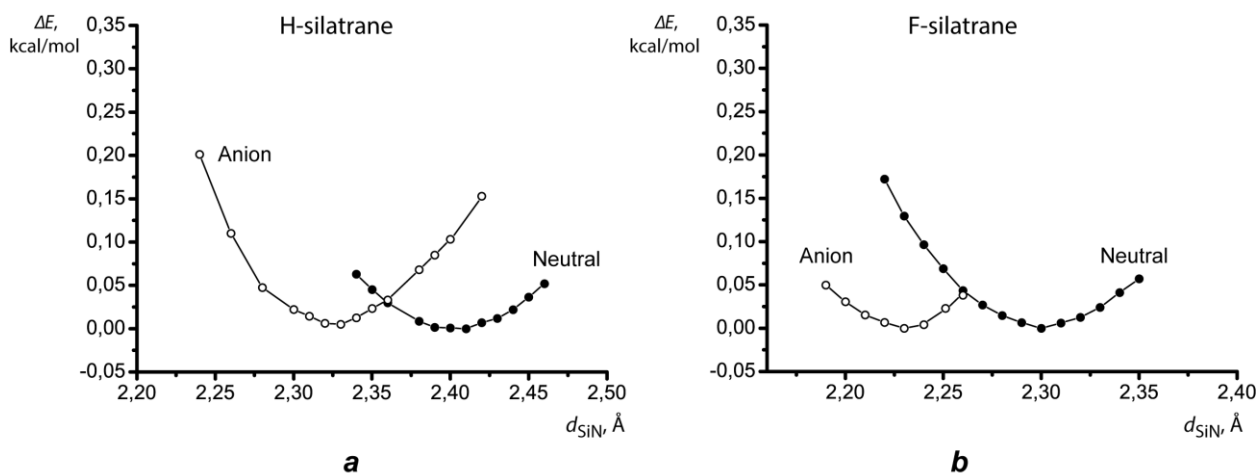


Figure S1. The CCSD(T)/B2(s) relative energies of H- and F-silatrane and their anions computed as functions of the Si...N distance (the values of the total energy in minima were set to zero). The energy surface scan with respect to $d_{\text{Si}\cdots\text{N}}$ was performed with increment of 0.01 Å and using the full MP2/B2(s) optimization of the remaining geometric parameters.

The $\Delta d_{\text{Si}\cdots\text{N}}$ values that were estimated at the CCSD(T)/B2(s) level of theory are ~ 0.08 Å for H-silatrane and ~ 0.07 Å for F-silatrane (Figure S1). They agree well with the $\Delta d_{\text{Si}\cdots\text{N}}$ values determined as the difference between the experimental lengths of the Si←N bond for neutral silatrane molecules and the MP2/B2(s) calculated bond lengths for their dipole-bound anions ($\Delta d_{\text{Si}\cdots\text{N}} = 0.106$ Å for H-silatrane and 0.101 Å for the F-silatrane). Note that the CCSD(T)/B2(s) method localizes a minimum at $d_{\text{Si}\cdots\text{N}} \sim 2.41$ Å for the neutral H-silatrane and at ~ 2.30 Å for F-silatrane. In contrast to the MP2/B2(s) method data, these $d_{\text{Si}\cdots\text{N}}$ values perfectly match the corresponding ED experimental data (see Table S2).

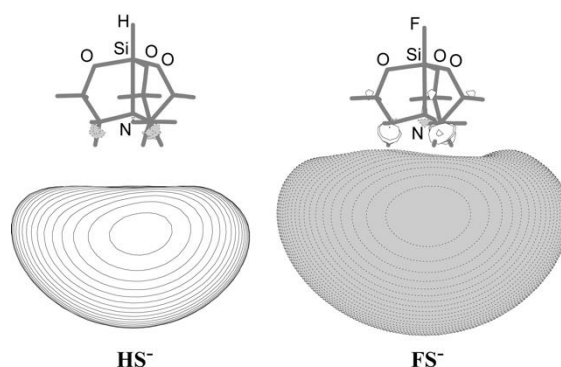


Figure S2. Singly occupied molecular orbitals of HS^- and FS^- at their MP2/B2(s) equilibrium geometries, plotted with 0.005 bohr^{-3/2} contour spacing.

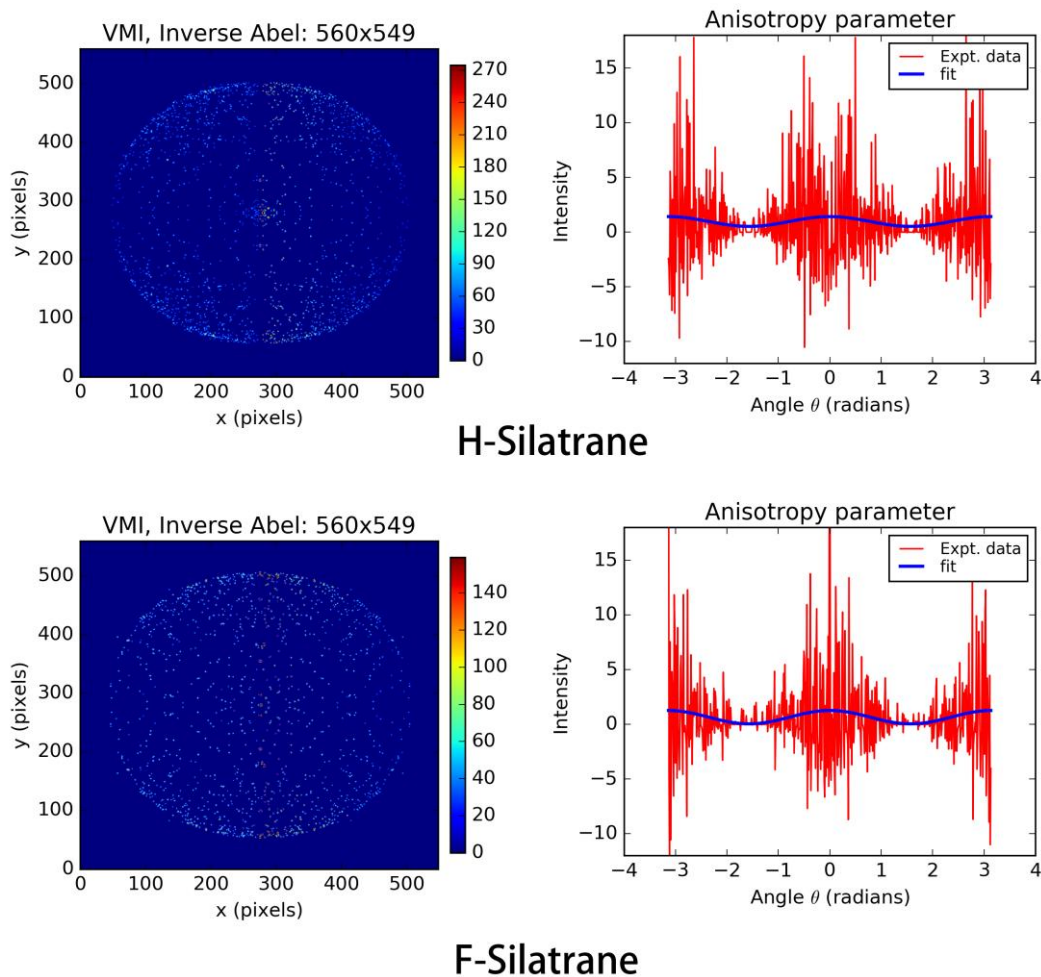


Figure S3. The velocity map photoelectron images and anisotropy parameters for H- and F-silatrane.

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Cartesian Coordinates**HS, MP2/B2(s)**

Si	0.000000000	0.000000000	1.347288000
N	0.000000000	0.000000000	-1.004574000
C	-0.456609000	1.350845000	-1.331165000
C	0.000000000	2.251604000	-0.183298000
O	-0.306955000	1.627861000	1.043375000
H	-0.081038000	1.695056000	-2.305734000
H	-1.550222000	1.342462000	-1.358914000
H	1.080726000	2.437552000	-0.252626000
H	-0.514209000	3.216301000	-0.224028000
C	1.398171000	-0.279988000	-1.331165000
C	1.949946000	-1.125802000	-0.183298000
O	1.563247000	-0.548100000	1.043375000
H	1.508481000	-0.777347000	-2.305734000
H	1.937717000	0.671301000	-1.358914000
H	1.570619000	-2.154712000	-0.252626000
H	3.042503000	-1.162833000	-0.224028000
C	-0.941562000	-1.070858000	-1.331165000
C	-1.949946000	-1.125802000	-0.183298000
O	-1.256292000	-1.079761000	1.043375000
H	-1.427443000	-0.917709000	-2.305734000
H	-0.387495000	-2.013763000	-1.358914000
H	-2.651345000	-0.282840000	-0.252626000
H	-2.528294000	-2.053469000	-0.224028000
H	0.000000000	0.000000000	2.813230000

HS⁻, MP2/B2(s)

Si	-0.004294000	0.000217000	-1.324023000
N	0.003547000	-0.001596000	0.975526000
C	-0.686797000	-1.247359000	1.321428000
C	-0.388730000	-2.229814000	0.189297000
O	-0.554949000	-1.570816000	-1.047126000
H	-0.381192000	-1.631966000	2.304174000
H	-1.761590000	-1.045047000	1.340367000

H	0.636818000	-2.614326000	0.277100000
H	-1.074631000	-3.081008000	0.230081000
C	1.428779000	0.022318000	1.315679000
C	2.125014000	0.776422000	0.183508000
O	1.632424000	0.307963000	-1.052664000
H	1.613037000	0.475798000	2.299347000
H	1.791284000	-1.009630000	1.329596000
H	1.945432000	1.856381000	0.276562000
H	3.205320000	0.607966000	0.219082000
C	-0.727948000	1.219752000	1.324023000
C	-1.734076000	1.450775000	0.197345000
O	-1.087671000	1.263123000	-1.042614000
H	-1.208095000	1.148729000	2.309691000
H	-0.015368000	2.049537000	1.337716000
H	-2.579518000	0.755329000	0.291274000
H	-2.127905000	2.470539000	0.238722000
H	-0.009284000	0.001671000	-2.792144000

FS, MP2/B2(s)

Si	0.000000000	0.000000000	1.065420000
N	0.000000000	0.000000000	-1.207297000
C	-0.455944000	1.351716000	-1.549896000
C	0.000000000	2.254895000	-0.404244000
O	-0.310319000	1.625324000	0.817803000
H	-0.075591000	1.681288000	-2.526202000
H	-1.549262000	1.343890000	-1.578934000
H	1.080107000	2.443443000	-0.470867000
H	-0.517312000	3.217408000	-0.442140000
C	1.398592000	-0.280999000	-1.549896000
C	1.952796000	-1.127448000	-0.404244000
O	1.562731000	-0.543918000	0.817803000
H	1.493834000	-0.775180000	-2.526202000
H	1.938474000	0.669755000	-1.578934000
H	1.576030000	-2.157121000	-0.470867000
H	3.045013000	-1.160699000	-0.442140000

C	-0.942648000	-1.070717000	-1.549896000
C	-1.952796000	-1.127448000	-0.404244000
O	-1.252412000	-1.081406000	0.817803000
H	-1.418242000	-0.906108000	-2.526202000
H	-0.389212000	-2.013645000	-1.578934000
H	-2.656137000	-0.286322000	-0.470867000
H	-2.527701000	-2.056709000	-0.442140000
F	0.000000000	0.000000000	2.681874000

FS⁻, MP2/B2(s)

Si	-0.000035000	-0.000029000	1.045081000
N	-0.000061000	-0.000027000	-1.177654000
C	-0.481759000	1.341262000	-1.537513000
C	-0.026220000	2.264405000	-0.409108000
O	-0.295449000	1.635583000	0.824809000
H	-0.116820000	1.657307000	-2.522955000
H	-1.574977000	1.314674000	-1.555279000
H	1.047010000	2.480702000	-0.497940000
H	-0.568798000	3.213087000	-0.445410000
C	1.402399000	-0.253468000	-1.537358000
C	1.974293000	-1.109430000	-0.408929000
O	1.564241000	-0.561861000	0.824985000
H	1.493745000	-0.727418000	-2.522854000
H	1.925859000	0.706632000	-1.555048000
H	1.625417000	-2.147181000	-0.497714000
H	3.067146000	-1.113454000	-0.445344000
C	-0.920833000	-1.087768000	-1.537522000
C	-1.947973000	-1.155066000	-0.408976000
O	-1.268649000	-1.073857000	0.824885000
H	-1.377030000	-0.929576000	-2.522923000
H	-0.351146000	-2.021184000	-1.555441000
H	-2.672202000	-0.333971000	-0.497503000
H	-2.497974000	-2.099444000	-0.445372000
F	-0.000182000	0.000084000	2.667535000

HS, CCSD/6-31++G(d,p)

Si	0.000000000	0.000000000	1.378894000
N	0.000000000	0.000000000	-1.037947000
C	-0.435244000	1.362661000	-1.347422000
C	-0.000076000	2.245916000	-0.177644000
O	-0.345133000	1.612676000	1.041545000
H	-0.036685000	1.723509000	-2.304094000
H	-1.524842000	1.368519000	-1.408791000
H	1.080973000	2.423405000	-0.211566000
H	-0.502004000	3.214535000	-0.214584000
C	1.397721000	-0.304398000	-1.347422000
C	1.945058000	-1.122892000	-0.177644000
O	1.569185000	-0.507444000	1.041545000
H	1.510946000	-0.829984000	-2.304094000
H	1.947594000	0.636293000	-1.408791000
H	1.558244000	-2.147852000	-0.211566000
H	3.034871000	-1.172519000	-0.214584000
C	-0.962477000	-1.058263000	-1.347422000
C	-1.944982000	-1.123023000	-0.177644000
O	-1.224052000	-1.105232000	1.041545000
H	-1.474260000	-0.893525000	-2.304094000
H	-0.422751000	-2.004812000	-1.408791000
H	-2.639217000	-0.275553000	-0.211566000
H	-2.532867000	-2.042015000	-0.214584000
H	0.000000000	0.000000000	2.842699000

HS⁻, CCSD/6-31++G(d,p)

Si	0.000000000	0.000000000	1.273418000
N	0.000000000	0.000000000	-0.908457000
C	-0.040609000	1.423822000	-1.294544000
C	0.721210000	2.179077000	-0.208397000
O	0.371137000	1.645107000	1.057685000
H	0.360147000	1.586090000	-2.299434000
H	-1.083823000	1.743749000	-1.293704000
H	1.803516000	2.096077000	-0.359231000

H	0.462798000	3.240570000	-0.230216000
C	1.253370000	-0.676742000	-1.294544000
C	1.526531000	-1.714125000	-0.208397000
O	1.239136000	-1.143967000	1.057685000
H	1.193521000	-1.104941000	-2.299434000
H	2.052042000	0.066744000	-1.293704000
H	0.913498000	-2.609929000	-0.359231000
H	2.575017000	-2.021080000	-0.230216000
C	-1.212761000	-0.747079000	-1.294544000
C	-2.247741000	-0.464952000	-0.208397000
O	-1.610273000	-0.501139000	1.057685000
H	-1.553668000	-0.481148000	-2.299434000
H	-0.968219000	-1.810493000	-1.293704000
H	-2.717014000	0.513852000	-0.359231000
H	-3.037815000	-1.219490000	-0.230216000
H	0.000000000	0.000000000	2.747575000

FS, CCSD/6-31++G(d,p)

Si	0.000000000	0.000000000	1.080974000
N	0.000000000	0.000000000	-1.211779000
C	-0.441267000	1.359869000	-1.553734000
C	0.001265000	2.259246000	-0.399802000
O	-0.321279000	1.622387000	0.822271000
H	-0.045828000	1.691550000	-2.520411000
H	-1.530957000	1.361963000	-1.607794000
H	1.078897000	2.452397000	-0.448816000
H	-0.515500000	3.219519000	-0.434053000
C	1.398314000	-0.297786000	-1.553734000
C	1.955932000	-1.130718000	-0.399802000
O	1.565668000	-0.532957000	0.822271000
H	1.487839000	-0.806086000	-2.520411000
H	1.944973000	0.644866000	-1.607794000
H	1.584389000	-2.160550000	-0.448816000
H	3.045935000	-1.163323000	-0.434053000
C	-0.957047000	-1.062083000	-1.553734000

C	-1.957196000	-1.128527000	-0.399802000
O	-1.244389000	-1.089429000	0.822271000
H	-1.442011000	-0.885463000	-2.520411000
H	-0.414016000	-2.006829000	-1.607794000
H	-2.663286000	-0.291846000	-0.448816000
H	-2.530435000	-2.056196000	-0.434053000
F	0.000000000	0.000000000	2.702511000

FS⁻, CCSD/6-31++G(d,p)

Si	0.000000000	0.000000000	1.008008000
N	0.000000000	0.000000000	-1.126987000
C	0.479845000	-1.342665000	-1.518624000
C	-0.000146000	-2.291296000	-0.423569000
O	0.182907000	-1.666693000	0.836178000
H	0.137366000	-1.618599000	-2.519560000
H	1.570753000	-1.321984000	-1.529607000
H	-1.056415000	-2.548000000	-0.561259000
H	0.574378000	-3.219842000	-0.442384000
C	-1.402705000	0.255774000	-1.518624000
C	-1.984247000	1.145775000	-0.423569000
O	-1.534852000	0.674944000	0.836178000
H	-1.470431000	0.690337000	-2.519560000
H	-1.930248000	-0.699320000	-1.529607000
H	-1.678426000	2.188882000	-0.561259000
H	-3.075654000	1.112495000	-0.442384000
C	0.922860000	1.086891000	-1.518624000
C	1.984394000	1.145521000	-0.423569000
O	1.351945000	0.991749000	0.836178000
H	1.333065000	0.928262000	-2.519560000
H	0.359495000	2.021304000	-1.529607000
H	2.734841000	0.359118000	-0.561259000
H	2.501276000	2.107347000	-0.442384000
F	0.000000000	0.000000000	2.647735000