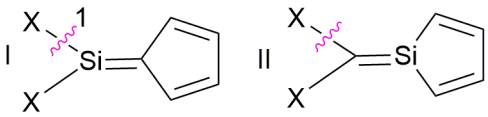
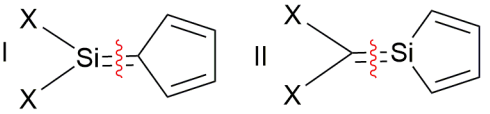
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Table S1. The energy decomposition analysis (kcal mol^{-1}) of the silapentafulvene isomers.



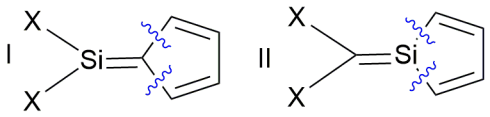
Substituent	CF_3	SiH_3	H	CN	Me	NH_2	Cl	OH	F
$\Delta E_{I\text{-}1\text{-}int}$	-85.7	-76.0	-97.7	-124.1	-101.4	-114.4	-105.8	-133.1	-152.2
$\Delta E_{I\text{-}1\text{-}pauli}$	185.6	112.3	51.1	190.8	174.2	440.5	323.2	332.0	357.5
$\Delta E_{I\text{-}1\text{-}elstat}$	-117.8	-86.8	-48.4	-115.0	-125.7	-238.0	-164.4	-174.6	-172.2
$\Delta E_{I\text{-}1\text{-}oi}$	-151.0	-99.1	-100.0	-198.4	-148.1	-315.3	-263.0	-289.4	-336.8
$\Delta E_{I\text{-}1\text{-}disp}$	-2.5	-2.4	-0.4	-1.4	-1.8	-1.6	-1.7	-1.1	-0.7
$\Delta E_{II\text{-}1\text{-}int}$	-118.0	-106.8	-124.3	-136.1	-115.7	-113.4	-88.9	-117.8	-127.2
$\Delta E_{II\text{-}1\text{-}pauli}$	276.0	188.7	87.9	295.3	249.0	805.8	364.8	535.0	503.9
$\Delta E_{II\text{-}1\text{-}elstat}$	-166.3	-130.1	-55.6	-155.0	-152.2	-345.7	-167.7	-247.8	-211.2
$\Delta E_{II\text{-}1\text{-}oi}$	-224.3	-163.0	-156.5	-274.9	-210.3	-571.2	-284.9	-403.6	-419.5
$\Delta E_{II\text{-}1\text{-}disp}$	-3.4	-2.8	-0.2	-1.5	-2.2	-2.2	-1.1	-1.4	-0.4
$\Delta\Delta E_{1\text{-}int}$	-32.3	-30.8	-26.6	-12.0	-14.3	1.0	16.9	15.3	25.1
$\Delta\Delta E_{1\text{-}pauli}$	90.4	76.4	36.8	104.5	74.8	365.2	41.6	203	146.3
$\Delta\Delta E_{1\text{-}elstat}$	-48.5	-43.3	-7.2	-40.0	-26.5	-107.7	-3.3	-73.2	-38.9
$\Delta\Delta E_{1\text{-}oi}$	-73.3	-63.9	-56.5	-76.5	-62.2	-255.9	-21.9	-114.2	-82.6
$\Delta\Delta E_{1\text{-}disp}$	-0.9	-0.1	0.3	0.0	-0.4	-0.6	0.6	-0.3	0.3

Table S2. The energy decomposition analysis (kcal mol^{-1}) of the silapentafulvene isomers.



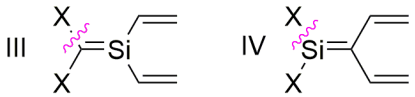
Substituent	CF_3	SiH_3	H	CN	Me	NH_2	Cl	OH	F
$\Delta E_{I\text{-}2\text{-}int}$	-134.4	-127.1	-136.2	-134.9	-145.7	-172.8	-142.7	-163.2	-155.7
$\Delta E_{I\text{-}2\text{-}pauli}$	217.9	223.9	214.3	213.6	223.9	243.4	211.9	211.0	194.0
$\Delta E_{I\text{-}2\text{-}elstat}$	-147.7	-149.2	-148.9	-147.4	-155.9	-170.7	-141.9	-145.4	-136.8
$\Delta E_{I\text{-}2\text{-}oi}$	-201.3	-198.4	-199.6	-198.4	-210.5	-242.5	-209.3	-226.0	-210.9
$\Delta E_{I\text{-}2\text{-}disp}$	-3.3	-3.5	-1.9	-2.8	-3.2	-3.0	-3.4	-2.8	-2.1
$\Delta E_{II\text{-}2\text{-}int}$	-146.1	-137.3	-124.4	-131.8	-129.9	-169.3	-124.6	-146.2	-135.6
$\Delta E_{II\text{-}2\text{-}pauli}$	225.7	257.9	215.9	248.2	238.1	162.5	250.4	170.5	196.1
$\Delta E_{II\text{-}2\text{-}elstat}$	-143.9	-164.6	-147.7	-142.4	-168.4	-116.2	-152.8	-123.3	-131.4
$\Delta E_{II\text{-}2\text{-}oi}$	-224.4	-227.7	-205.5	-235.2	-197.0	-212.5	-219.8	-191.0	-199.0
$\Delta E_{II\text{-}2\text{-}disp}$	-3.4	-2.9	-0.2	-2.3	-2.6	-3.1	-2.3	-2.4	-1.3
$\Delta\Delta E_{2\text{-}int}$	-11.7	-10.2	11.8	3.1	15.8	3.4	18.2	17.1	20.1
$\Delta\Delta E_{2\text{-}pauli}$	7.8	34.0	1.7	34.5	14.2	-81.0	38.5	-40.5	2.1
$\Delta\Delta E_{2\text{-}elstat}$	3.8	-15.4	1.2	5.0	-12.4	54.5	-10.9	22.1	5.4
$\Delta\Delta E_{2\text{-}oi}$	-23.1	-29.4	-5.8	-36.8	13.4	30.0	-10.5	35.0	11.9
$\Delta\Delta E_{2\text{-}disp}$	-0.1	0.5	1.7	0.5	0.6	-0.2	1.1	0.4	0.8

Table S3. The energy decomposition analysis (kcal mol^{-1}) of the silapentafulvene isomers.



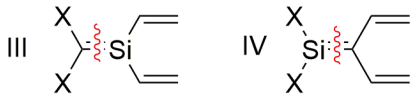
Substituent	CF_3	SiH_3	H	CN	Me	NH_2	Cl	OH	F
$\Delta E_{I\text{-}3\text{-}int}$	-276.2	-276.4	-276.1	-277.4	-274.2	-266.5	-267.1	-264.9	-265.4
$\Delta E_{I\text{-}3\text{-}pauli}$	1091.4	1140.7	1138.2	1100.4	1157.7	1160.1	1096.2	1134.5	1083.8
$\Delta E_{I\text{-}3\text{-}elstat}$	-471.6	-491.1	-490.7	-475.3	-498.2	-500.4	-477.4	-492.0	-475.5
$\Delta E_{I\text{-}3\text{-}oi}$	-893.2	-923.1	-921.8	-900.2	-931.2	-923.8	-883.4	-905.1	-871.8
$\Delta E_{I\text{-}3\text{-}disp}$	-2.7	-3.0	-1.8	-2.4	-2.6	-2.3	-2.6	-2.2	-1.9
$\Delta E_{II\text{-}3\text{-}int}$	-213.6	-212.2	-204.3	-200.8	-194.6	-181.8	-183.2	-176.8	-177.4
$\Delta E_{II\text{-}3\text{-}pauli}$	517.9	528.7	532.9	523.0	543.5	465.3	527.2	452.1	520.2
$\Delta E_{II\text{-}3\text{-}elstat}$	-282.3	-290.9	-292.0	-282.2	-297.7	-284.5	-282.6	-270.5	-280.3
$\Delta E_{II\text{-}3\text{-}oi}$	-446.7	-447.5	-443.8	-437.6	-438.5	-359.9	-425.7	-356.3	-416.0
$\Delta E_{II\text{-}3\text{-}disp}$	-2.4	-2.5	-1.4	-1.9	-1.9	-2.7	-2.0	-2.2	-1.4
$\Delta\Delta E_{3\text{-}int}$	62.6	64.2	71.8	76.7	79.6	84.7	84.0	88.1	88.0
$\Delta\Delta E_{3\text{-}pauli}$	-573.5	-612.1	-605.3	-579.4	-614.3	-694.8	-569	-682.4	-563.5
$\Delta\Delta E_{3\text{-}elstat}$	189.3	200.1	198.7	193.1	200.5	216.0	194.8	221.5	195.2
$\Delta\Delta E_{3\text{-}oi}$	446.5	475.7	478.0	462.6	492.7	563.9	457.7	548.8	455.8
$\Delta\Delta E_{3\text{-}disp}$	0.3	0.4	0.3	0.5	0.6	-0.4	0.6	0.0	0.4

Table S4. The energy decomposition analysis (kcal mol^{-1}) of the silene isomers.



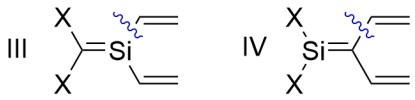
Substituent	CF_3	SiH_3	H	CN	Me	NH_2	Cl	OH	F
$\Delta E_{III\text{-}1\text{-}int}$	-81.1	-78.4	-100.6	-125.2	-102.9	-108.8	-103.0	-123.8	-141.5
$\Delta E_{III\text{-}1\text{-}pauli}$	198.2	135.7	88.9	247.6	217.0	465.1	282.0	399.2	376.8
$\Delta E_{III\text{-}1\text{-}elstat}$	-118.0	-99.8	-59.9	-139.4	-144.3	-248.3	-156.7	-205.8	-183.0
$\Delta E_{III\text{-}1\text{-}oi}$	-158.4	-111.83	-129.1	-231.7	-173.5	-323.9	-226.3	-315.8	-334.5
$\Delta E_{III\text{-}1\text{-}disp}$	-2.9	-2.5	-0.5	-1.6	-2.0	-1.8	-2.0	-1.4	-0.8
$\Delta E_{IV\text{-}1\text{-}int}$	-112.0	-106.7	-124.7	-139.7	-115.4	-109.0	-90.0	-109.2	-126.6
$\Delta E_{IV\text{-}1\text{-}pauli}$	284.8	192.6	88.5	315.3	249.0	807.2	362.9	586.0	456.0
$\Delta E_{IV\text{-}1\text{-}elstat}$	-172.0	-133.8	-57.3	-167.1	-153.0	-346.3	-168.6	-254.0	-189.0
$\Delta E_{IV\text{-}1\text{-}oi}$	-228.9	-162.8	-155.7	-286.1	-208.8	-567.6	-282.8	-439.7	-393.1
$\Delta E_{IV\text{-}1\text{-}disp}$	-3.9	-2.8	-0.2	-1.8	-2.6	-2.2	-1.5	-1.5	-0.6
$\Delta\Delta E_{1\text{-}int}$	-30.9	-28.3	-24.1	-14.5	-12.5	-0.2	13.0	14.6	14.9
$\Delta\Delta E_{1\text{-}pauli}$	86.6	56.9	-0.4	67.7	32.0	342.1	80.9	186.8	79.2
$\Delta\Delta E_{1\text{-}elstat}$	-54.0	-34.0	2.6	-27.7	-8.7	-98.0	-11.9	-48.2	-6.0
$\Delta\Delta E_{1\text{-}oi}$	-70.5	-50.97	-26.6	-54.4	-35.3	-243.7	-56.5	-123.9	-58.6
$\Delta\Delta E_{1\text{-}disp}$	-1.0	-0.3	0.3	-0.2	-0.6	-0.4	0.5	-0.1	0.2

Table S5. The energy decomposition analysis (kcal mol^{-1}) of the silene isomers.



Substituent	CF_3	SiH_3	H	CN	Me	NH_2	Cl	OH	F
$\Delta E_{III\text{-}2\text{-}int}$	-125.7	-116.9	-125.3	-126.9	-132.0	-149.3	-130.1	-144.3	-140.9
$\Delta E_{III\text{-}2\text{-}pauli}$	231.8	238.0	228.4	224.5	238.2	239.4	224.6	216.7	211.9
$\Delta E_{III\text{-}2\text{-}elstat}$	-158.0	-156.2	-156.0	-153.3	-161.3	-162.5	-148.3	-150.8	-150.7
$\Delta E_{III\text{-}2\text{-}oi}$	-195.5	-195.1	-195.7	-195.0	-205.5	-223.0	-202.5	-207.5	-199.8
$\Delta E_{III\text{-}2\text{-}disp}$	-4.0	-3.6	-1.9	-3.1	-3.4	-3.3	-3.9	-2.8	-2.3
$\Delta E_{IV\text{-}2\text{-}int}$	-156.7	-146.2	-145.1	-143.1	-136.1	-163.2	-134.0	-137.6	-143.4
$\Delta E_{IV\text{-}2\text{-}pauli}$	220.8	251.2	213.3	246.6	236.7	184.4	250.5	220.9	197.4
$\Delta E_{IV\text{-}2\text{-}elstat}$	-145.6	-164.0	-150.0	-146.7	-169.8	-141.2	-156.6	-157.0	-138.1
$\Delta E_{IV\text{-}2\text{-}oi}$	-227.6	-229.9	-207.1	-239.9	-199.5	-202.8	-224.7	-199.0	-200.9
$\Delta E_{IV\text{-}2\text{-}disp}$	-4.3	-3.6	-1.3	-3.1	-3.4	-3.5	-3.2	-2.5	-1.8
$\Delta\Delta E_{2\text{-}int}$	-31.0	-29.3	-19.8	-16.2	-4.1	-13.9	-3.9	6.7	-2.5
$\Delta\Delta E_{2\text{-}pauli}$	-11.0	13.2	-15.1	22.1	-1.5	-55	25.9	4.2	-14.5
$\Delta\Delta E_{2\text{-}elstat}$	12.4	-7.8	6.0	6.6	-8.5	21.3	-8.3	-6.2	12.6
$\Delta\Delta E_{2\text{-}oi}$	-32.1	-34.8	-11.4	-44.9	6.0	20.2	-22.2	8.5	-1.1
$\Delta\Delta E_{2\text{-}disp}$	-0.3	0.0	0.6	0.0	0.0	-0.2	0.7	0.3	0.5

Table S6. The energy decomposition analysis (kcal mol^{-1}) of the silene isomers.



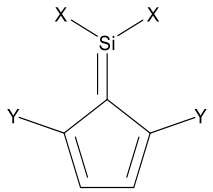
Substituent	CF_3	SiH_3	H	CN	Me	NH_2	Cl	OH	F
$\Delta E_{III\text{-}3\text{-}int}$	-125.9	-126.7	-129.4	-131.1	-130.3	-128.3	-128.4	-128.9	-124.9
$\Delta E_{III\text{-}3\text{-}pauli}$	359.6	315.3	343.1	368.1	384.8	538.8	511.2	509.8	443.2
$\Delta E_{III\text{-}3\text{-}elstat}$	-199.2	-183.5	-196.1	-203.2	-211.7	-253.1	-240.6	-244.4	-225.2
$\Delta E_{III\text{-}3\text{-}oi}$	-282.5	-255.0	-273.5	-292.8	-299.9	-410.7	-395.5	-391.1	-340.0
$\Delta E_{III\text{-}3\text{-}disp}$	-3.8	-3.6	-2.9	-3.4	-3.4	-3.3	-3.6	-3.1	-3.0
$\Delta E_{IV\text{-}3\text{-}int}$	-107.6	-104.8	-105.8	-109.9	-106.4	-88.7	-108.2	-106.8	-106.3
$\Delta E_{IV\text{-}3\text{-}pauli}$	187.9	191.4	184.6	194.8	193.2	221.0	240.1	268.1	269.7
$\Delta E_{IV\text{-}3\text{-}elstat}$	-134.5	-135.2	-132.6	-137.2	-136.5	-136.6	-154.7	-165.4	-163.7
$\Delta E_{IV\text{-}3\text{-}oi}$	-157.5	-157.6	-155.2	-164.2	-160.0	-169.9	-190.6	-206.9	-209.9
$\Delta E_{IV\text{-}3\text{-}disp}$	-3.5	-3.4	-2.5	-3.0	-3.1	-3.3	-3.0	-2.6	-2.4
$\Delta\Delta E_{3\text{-}int}$	18.3	21.9	23.6	21.2	23.9	39.6	20.2	22.1	18.6
$\Delta\Delta E_{3\text{-}pauli}$	-171.7	-123.9	-158.5	-173.3	-191.6	-317.8	-271.1	-241.7	-173.5
$\Delta\Delta E_{3\text{-}elstat}$	64.7	48.3	63.5	66.0	75.2	116.5	85.9	79.0	61.5
$\Delta\Delta E_{3\text{-}oi}$	125.0	97.4	118.3	128.6	139.9	240.8	204.9	184.2	130.1
$\Delta\Delta E_{3\text{-}disp}$	0.3	0.2	0.4	0.4	0.3	0.0	0.6	0.5	0.6

The interaction energies are divided into four parts:

$$\Delta E_{int} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{orb} + \Delta E_{disp} \quad (1)$$

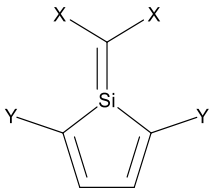
The bonding energy between the interacting fragments can be decomposed in the following way. In the first step, a calculation is carried out on the molecule in which only the occupied orbitals of the fragments are used as a basis. The calculation yields the bonding energy, ΔE_{steric}, which can be further decomposed into ΔE_{elstat}, the electrostatic interactions and ΔE_{Pauli}, the Pauli repulsive orbital interactions. The frozen geometry of the entire molecule are superimposed without electronic relaxation to yield the quasi-classical electrostatic attraction ΔE_{elstat}. The ΔE_{elstat} accounts for the classical electrostatic interaction between the unperturbed charge distributions of the prepared fragments. The ΔE_{Pauli} is calculated when the product wave function becomes antisymmertrized and renormalized, it comprises the destabilizing interactions between occupied orbitals and is responsible for the steric repulsion. In the second step, the orbital interaction ΔE_{oi} is acquired by calculating the occupied orbitals as well as virtual orbitals on the fragments. At last, the term ΔE_{disp} corresponds to the dispersion corrections which are introduced by Grimme and co-workers. Finally, the interaction energy can be described by the equation 1.

Table S7. The $NICS(1)_{zz}$ values and ΔE_{ST} values of the substituted 6-silapentafulvenes.



X	Y	ΔE_{ST} (kcal mol^{-1})	$NICS(1)_{zz}$ (ppm)
CF_3	H	15.6	-5.4
SiH_3	H	25.0	-7.2
H	H	25.2	-10.5
CN	H	17.2	-0.4
Me	H	28.6	-15.8
NH_2	H	32.5	-23.6
Cl	H	18.4	-13.6
OH	H	24.4	-22.1
F	H	15.4	-18.7
CF_3	NH_2	-6.2	24.4
SiH_3	NH_2	8.7	4.7
H	NH_2	5.4	11.8
CN	NH_2	-6.9	35.7
Me	NH_2	11.5	-6.1
NH_2	NH_2	15.6	-19.7
Cl	NH_2	-4.6	1.6
OH	NH_2	6.8	-13.2
F	NH_2	-7.5	-2.6

Table S8. The $NICS(1)_{zz}$ values and ΔE_{ST} values of the substituted 5-silapentafulvenes.



X	Y	ΔE_{ST} (kcal mol^{-1})	$NICS(1)_{zz}$ (ppm)
CF_3	H	38.9	8.8
SiH_3	H	38.4	5.1
H	H	34.1	1.3
CN	H	66.5	8.9
Me	H	31.0	-1.8
NH_2	H	33.3	-10.4
Cl	H	24.9	1.3
OH	H	29.7	-9.7
F	H	24.8	-4.0
CF_3	NH_2	17.9	23.7
SiH_3	NH_2	22.4	18.2
H	NH_2	28.2	12.6
CN	NH_2	14.1	25.4
Me	NH_2	30.7	8.2
NH_2	NH_2	48.8	-0.6
Cl	NH_2	24.9	11.6
OH	NH_2	21.1	6.0
F	NH_2	18.4	7.0

Table S9. The bond lengths (Å), ΣαSi, ΔE (kcal mol^{-1}) and dipole moment (Debye) of the silapentafulvene isomers **I** and **II**

Compound	Dipole moment (Deybe)	ΔE (kcal $mole^{-1}$;relative to the isomers I)	Symmetry	ΣαSi	Bond length of Si=C (Å)
I-CF_3	-1.4	0.0	C_2	360.0°	1.724
II-CF_3	-6.4	-19.4	C_2	360.0°	1.733
I-SiH_3	2.2	0.0	C_{2v}	360.0°	1.751
II-SiH_3	-2.9	-9.0	C_{2v}	360.0°	1.718
I-H	2.3	0.0	C_{2v}	360.0°	1.732
II-H	-1.2	-1.0	C_{2v}	360.0°	1.713
I-CN	-2.9	0.0	C_{2v}	360.0°	1.725
II-CN	-8.2	8.3	C_{2v}	360.0°	1.749
I-Me	4.5	0.0	C_{2v}	360.0°	1.736
II-Me	0.3	16.5	C_{2v}	360.0°	1.734
I-NH_2	6.5	0.0	C_2	360.0°	1.731
II-NH_2	6.6	43.3	C_1	291.8°	1.926
I-Cl	1.5	0.0	C_{2v}	360.0°	1.719
II-Cl	-2.8	63.3	C_{2v}	360.0°	1.737
I-OH	6.3	0.0	C_{2v}	360.0°	1.722
II-OH	3.1	63.9	C_2	309.9°	1.849
I-F	1.0	0.0	C_{2v}	360.0°	1.706
II-F	-2.3	85.2	C_S	360.0°	1.747

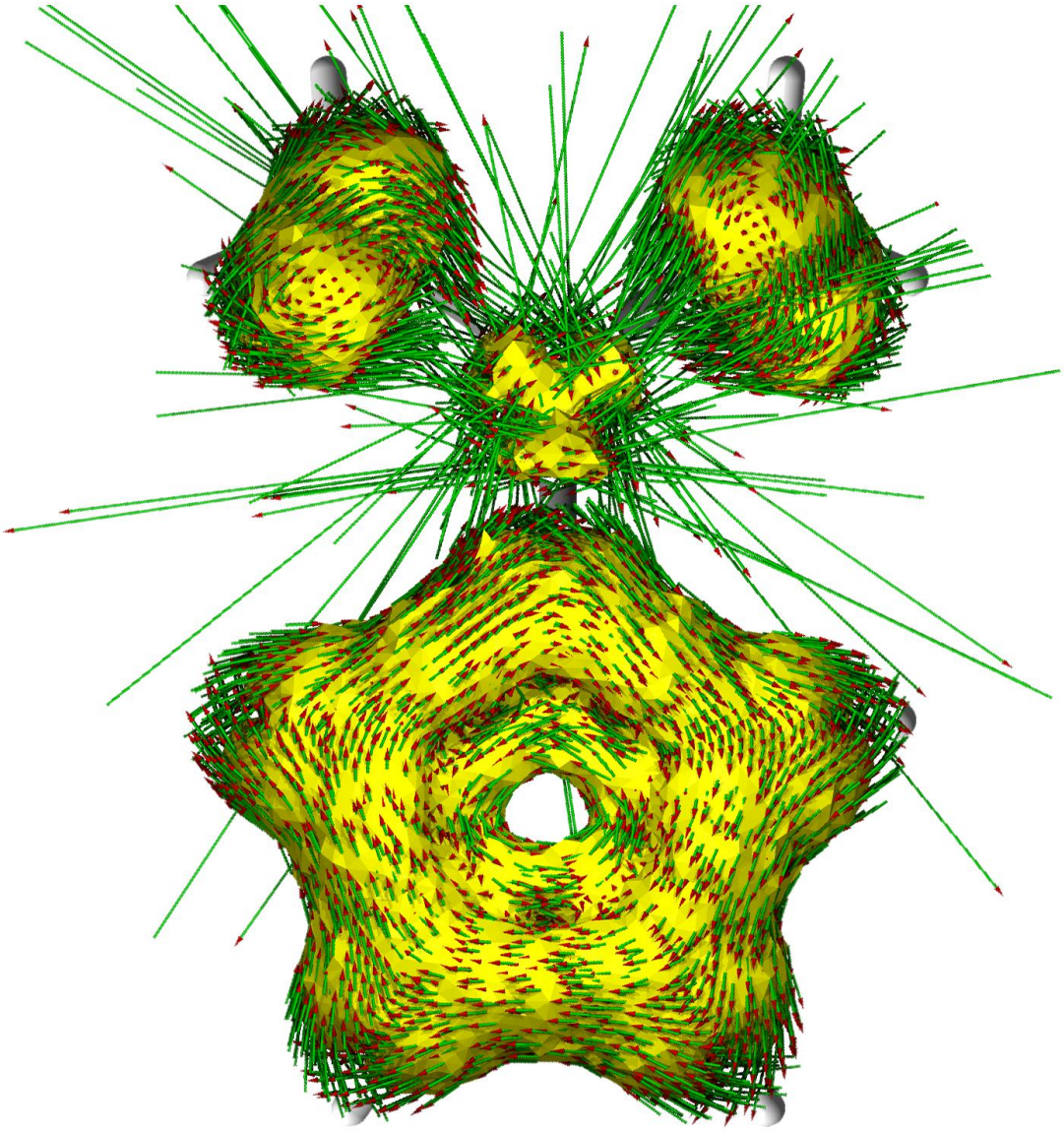


Figure S1. ACID calculations with an isovalue of 0.025 a.u. on **I-NH$_2$**.

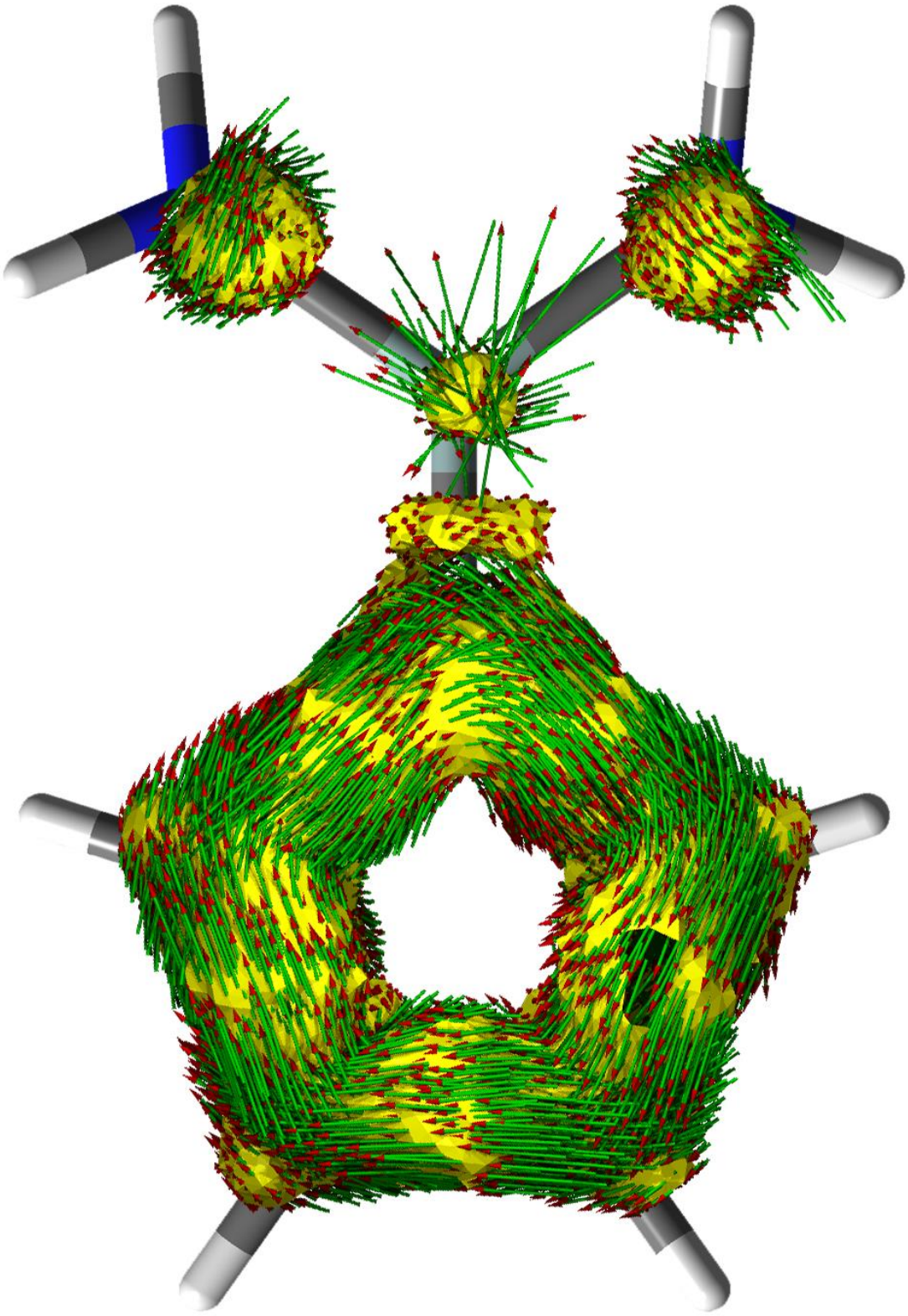


Figure S2. ACID calculations with an isovalue of 0.025 a.u. on π orbitals of **I-NH$_2$**.

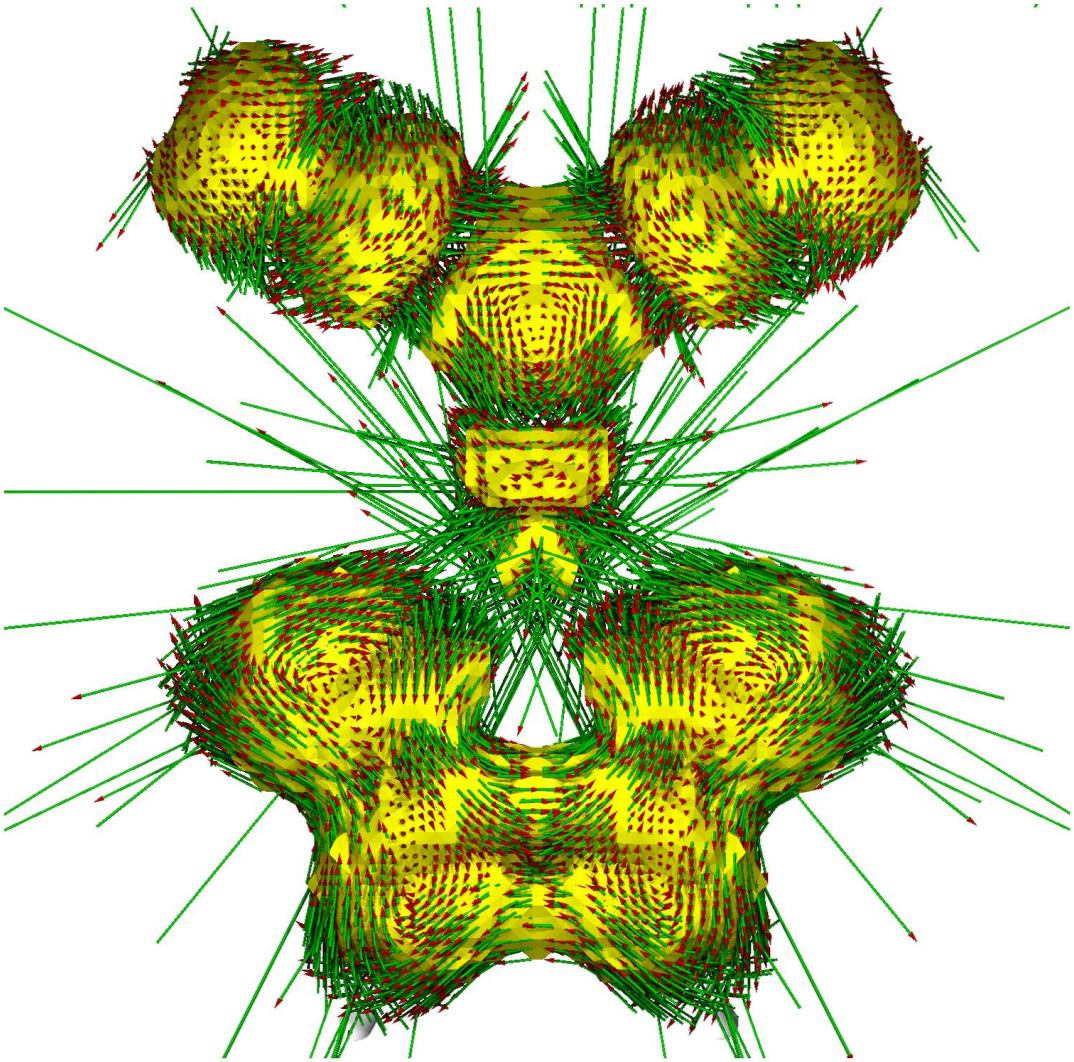


Figure S3. ACID calculations with an isovalue of 0.025 a.u. on **II-CN**.

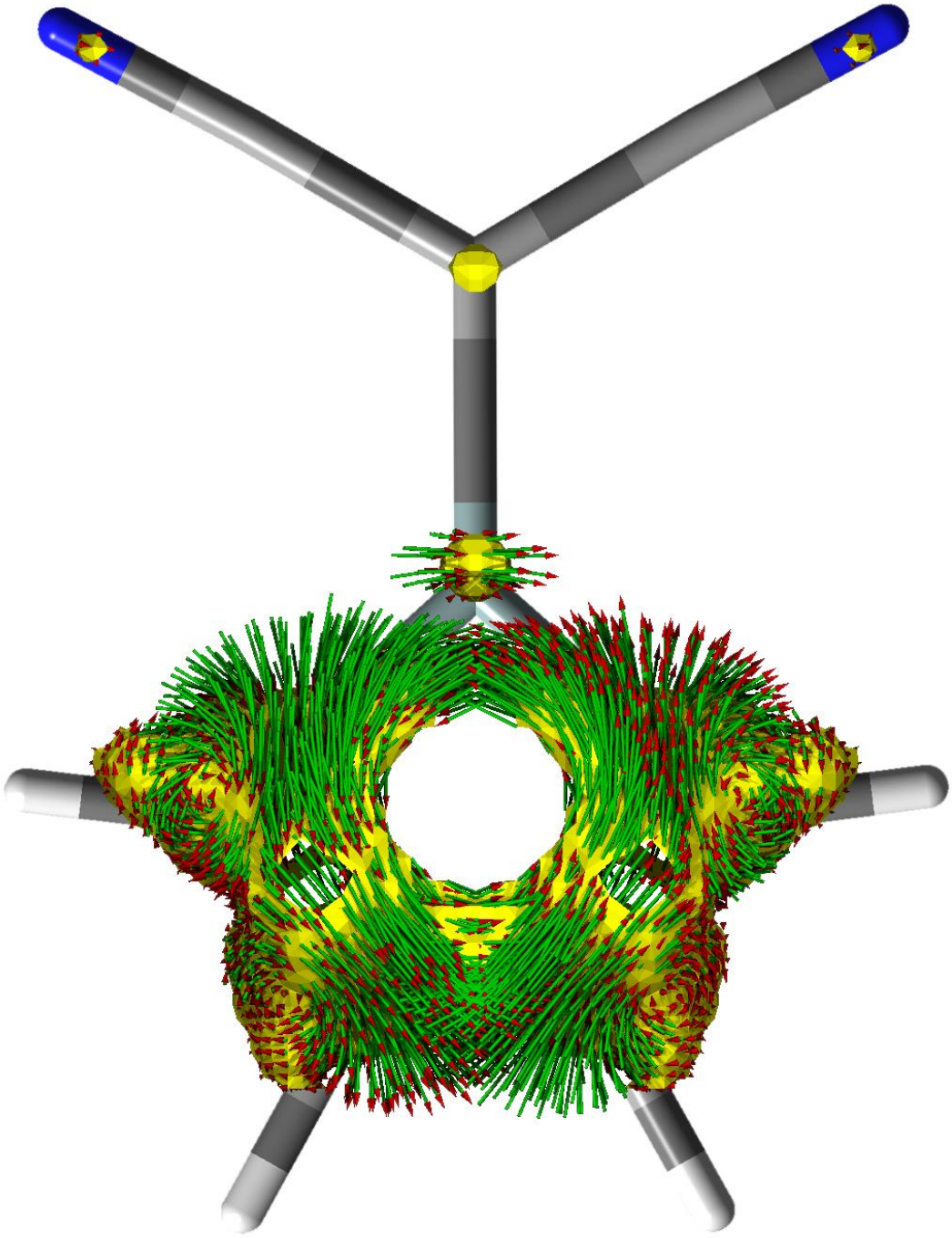


Figure S4. ACID calculations with an isovalue of 0.025 a.u. on π orbitals of **II-CN**.

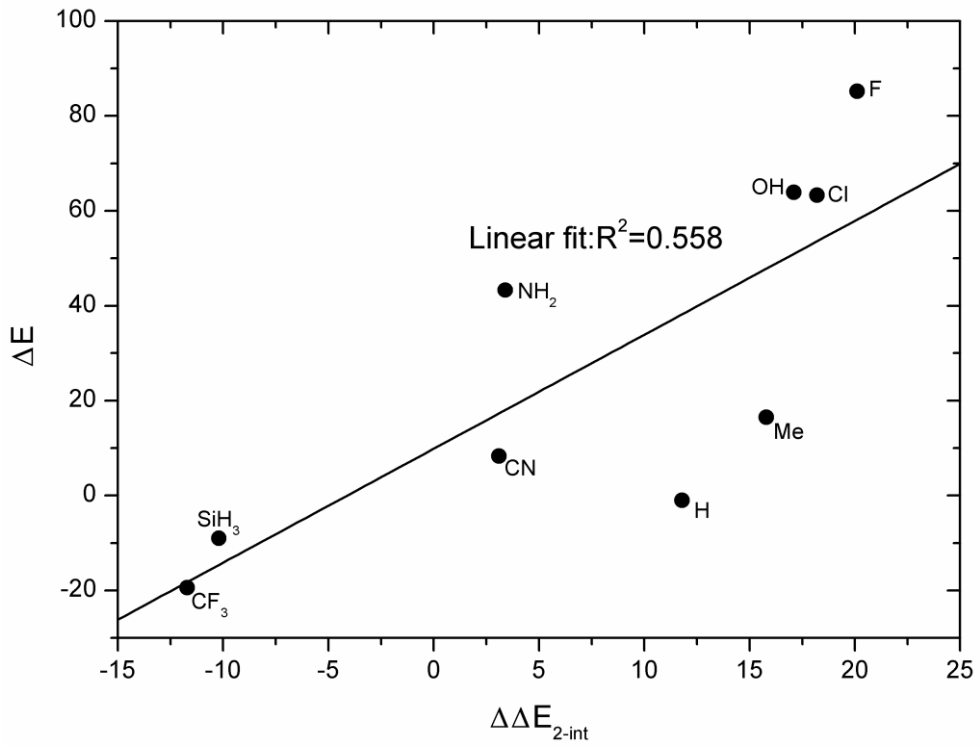


Figure S5. Plot of $\Delta\Delta E_{2\text{-int}}$ *versus* ΔE of the silapentafulvene isomers **I** and **II** (kcal mol^{-1}).

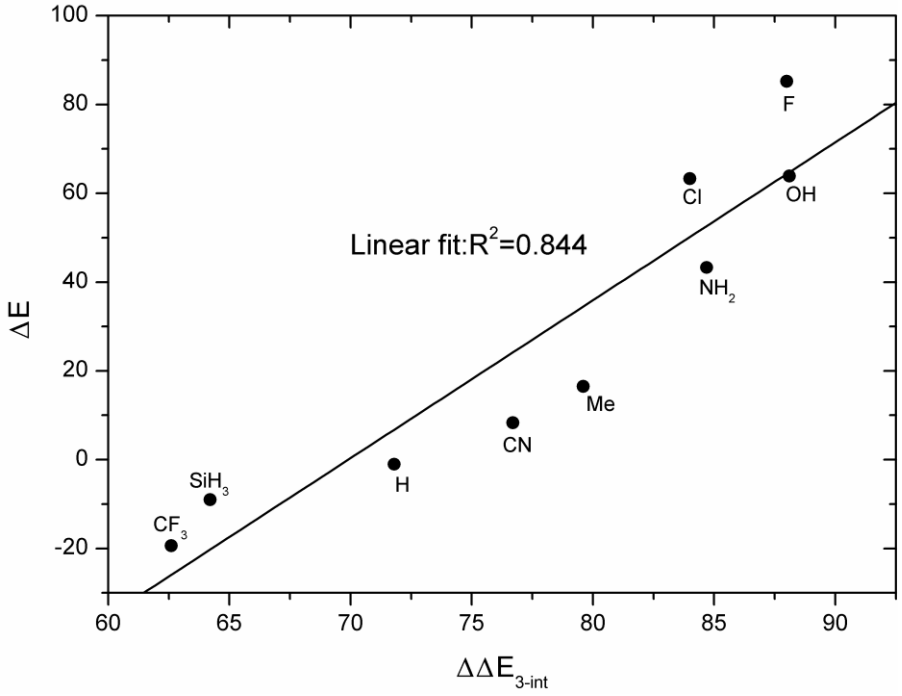


Figure S6. Plot of $\Delta\Delta E_{3\text{-int}}$ *versus* ΔE of the silapentafulvene isomers **I** and **II** (kcal mol^{-1}).

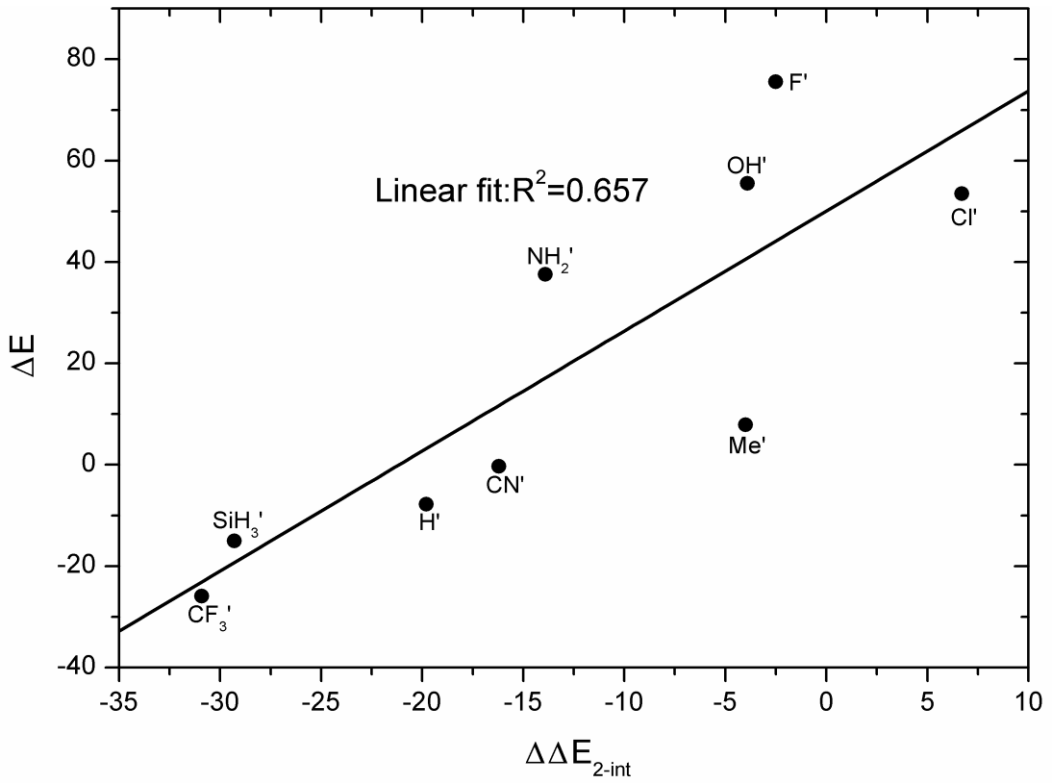


Figure S7. Plot of $\Delta\Delta E_{2\text{-int}}$ *versus* ΔE of the silene isomers **III** and **IV** (kcal mol^{-1}).

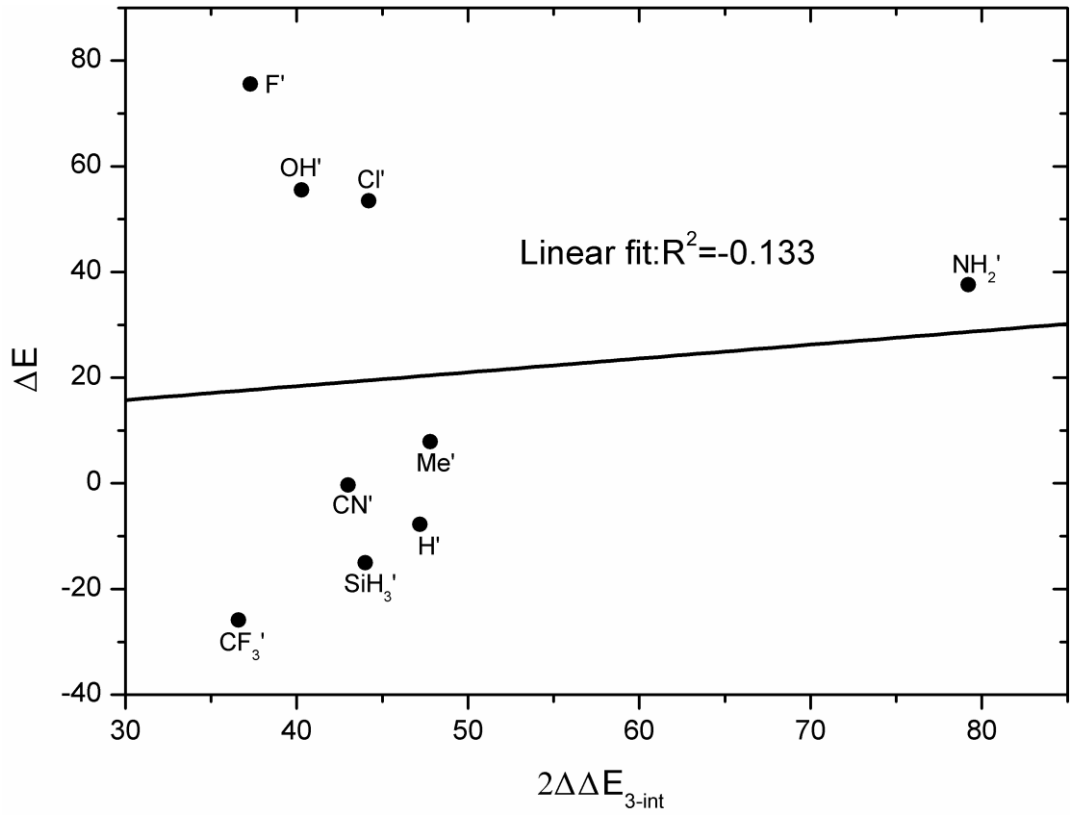


Figure S8. Plot of $2\Delta\Delta E_{3\text{-int}}$ *versus* ΔE of the silene isomers **III** and **IV** (kcal mol^{-1}).

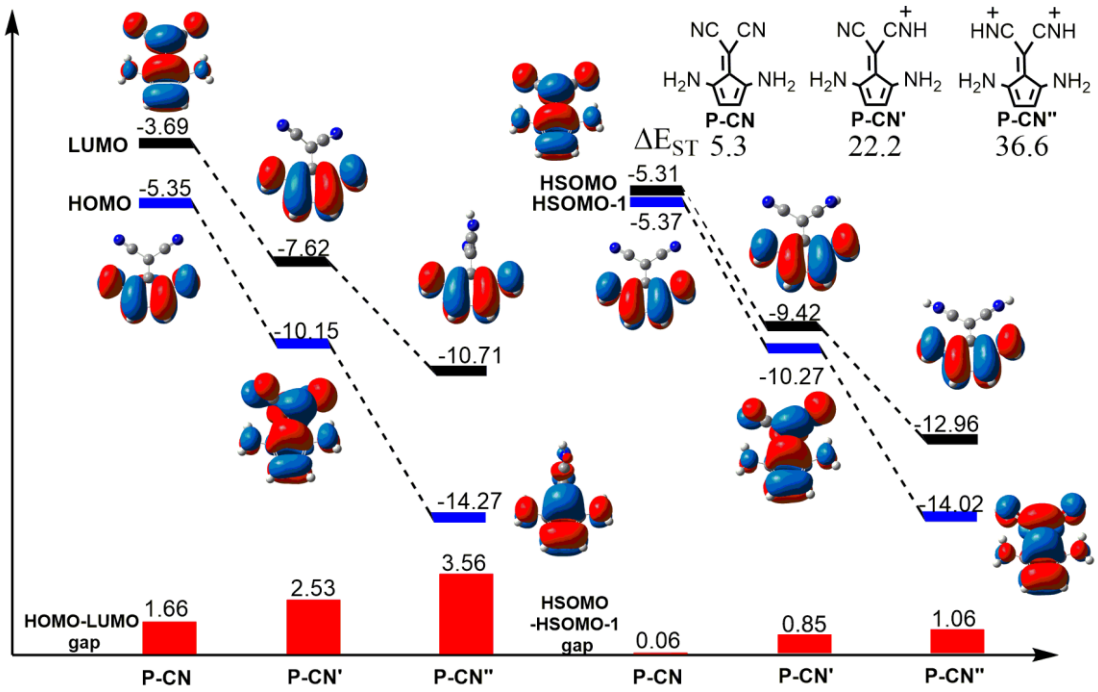


Figure S9. The HOMO, LUMO, HOMO-LUMO gap, HSOMO, HSOMO, HSOMO-HSOMO-1 gap (eV) and ΔE_{ST} (kcal mol^{-1}) of **P-CN**, **P-CN'** and **P-CN''** in its singlet and triplet states.

Cartesian Coordinates

I-CF_3

E = -1155.5242315 a.u.

C	2.47568100	-1.17788500	-0.01085300
H	2.14047000	-2.20355200	-0.02340600
C	3.75957400	-0.73113200	-0.00702500
H	4.64612500	-1.35053400	-0.01364600
C	2.47590500	1.17789300	0.01095300
H	2.14090200	2.20362500	0.02362400
C	3.75970800	0.73087300	0.00689800
H	4.64637600	1.35011300	0.01332900
C	1.60063900	0.00011400	0.00010100
C	-1.22642000	1.59638300	-0.00226400
C	-1.22643700	-1.59640500	0.00223300
Si	-0.12345800	-0.00001900	0.00014500
F	-2.18876700	1.53459600	0.94688200
F	-0.49017900	2.70233100	0.23712600
F	-1.85184400	1.77718800	-1.18800700
F	-2.18847800	-1.53443000	-0.94720000
F	-1.85228100	-1.77702800	1.18782800
F	-0.49037900	-2.70248300	-0.23687300

I-SiH_3

E = -1063.0631500 a.u.

C	1.87840500	-1.16977200	-0.00014700
H	1.54658100	-2.19785500	-0.00032700
C	3.16840800	-0.72954700	-0.00019500
H	4.05483100	-1.34999900	-0.00046600
C	1.87838100	1.16981700	0.00022400
H	1.54653000	2.19789200	0.00044300
C	3.16839700	0.72962900	0.00004800
H	4.05480600	1.35010200	0.00006500
C	0.99876900	0.00001800	0.00007400
Si	-0.75256000	-0.00000100	0.00020800
Si	-1.93079500	-2.03430000	0.00000900
H	-2.79824000	-2.10720300	-1.20461200
H	-0.98127400	-3.17377300	0.00047100
H	-2.79888700	-2.10667400	1.20420100
Si	-1.93091800	2.03424000	-0.00015500
H	-2.79897200	2.10686800	1.20404400
H	-0.98137800	3.17370500	0.00008700
H	-2.79833200	2.10693700	-1.20480600

I-H

E = -482.6001580 a.u.

C	0.58798700	-1.17108400	-0.00024000
H	0.25346500	-2.19872200	-0.00031300
C	1.87789400	-0.72880300	0.00042200
H	2.76420200	-1.34923000	0.00063700
C	0.58797000	1.17107800	0.00027500
H	0.25343200	2.19871100	0.00037300
C	1.87788300	0.72881800	-0.00045200
H	2.76418300	1.34925700	-0.00071300
C	-0.28779500	-0.00001100	0.00003500
Si	-2.02026300	-0.00000100	-0.00001300
H	-2.80763000	-1.24764400	-0.00022500
H	-2.80760500	1.24765600	0.00018800

I-CN

E = -666.7102746 a.u.

C	1.68928100	-1.17790400	0.00043700
H	1.35170500	-2.20360300	0.00105400
C	2.97393300	-0.73258100	-0.00022500
H	3.86080400	-1.35133600	-0.00027300
C	1.68927100	1.17788400	-0.00042000
H	1.35168800	2.20358000	-0.00102300
C	2.97392700	0.73257200	0.00020700
H	3.86079300	1.35133500	0.00023300
C	0.81995700	-0.00001500	0.00001900
Si	-0.90506100	-0.00000300	-0.00000400
C	-1.91508800	-1.50835300	-0.00009500
C	-1.91505200	1.50837100	0.00009400
N	-2.54656700	-2.47809500	-0.00018600
N	-2.54650800	2.47812800	0.00018000

I-Me

E = -561.0569820 a.u.

C	1.34879000	-1.16644000	-0.00038300
H	1.02169100	-2.19698000	-0.00078600
C	2.64392300	-0.72467800	-0.00013200
H	3.52860000	-1.34779900	-0.00033400
C	1.34833000	1.16600800	0.00035100
H	1.02085500	2.19642000	0.00070900
C	2.64363000	0.72478000	0.00018900
H	3.52806000	1.34825000	0.00044500
C	0.47220500	-0.00045200	-0.00009100
Si	-1.26385200	-0.00010400	-0.00000600
C	-2.27071000	-1.57613700	0.00033000
H	-1.62032200	-2.45248100	0.00085400
H	-2.91763300	-1.62615800	0.88156700
H	-2.91775100	-1.62717800	-0.88073900
C	-2.26931900	1.57677400	-0.00032600
H	-2.91630000	1.62815500	0.88078800
H	-1.61805200	2.45244200	-0.00059300
H	-2.91631200	1.62766400	-0.88146600

I-NH_2

E = -593.1588429 a.u.

C	-1.32528100	-1.14988700	0.17963900
H	-0.99913400	-2.16573700	0.35827500
C	-2.62818300	-0.70968500	0.11178400
H	-3.51000000	-1.32798300	0.21628400
C	-1.32529100	1.14991500	-0.17956000
H	-0.99914900	2.16578000	-0.35812600
C	-2.62818900	0.70967700	-0.11187300
H	-3.51001000	1.32795100	-0.21647300
C	-0.46068100	0.00002700	0.00009800
Si	1.27005100	0.00000300	-0.00000100
N	2.23968000	-1.37567100	-0.18921400
H	1.86229900	-2.24670100	-0.53107200
H	3.18127600	-1.46180300	0.16173200
N	2.23975100	1.37563400	0.18917100
H	1.86241300	2.24669000	0.53101200
H	3.18132000	1.46173600	-0.16185600

I-Cl

E = -1400.8281590 a.u.

C	1.81905300	-1.17436500	-0.00037700
H	1.48394300	-2.20095000	-0.00059600
C	3.10938100	-0.72558900	-0.00038800
H	3.99383700	-1.34822400	-0.00073800
C	1.81904500	1.17435300	0.00036900
H	1.48392900	2.20093700	0.00058900
C	3.10937700	0.72558500	0.00037600
H	3.99382900	1.34822600	0.00071200
C	0.95438700	-0.00000900	0.00004200
Si	-0.76510300	-0.00000300	-0.00000200
Cl	-1.91505800	-1.67922600	0.00022800
Cl	-1.91503300	1.67923800	-0.00023300

I-OH

E = -632.8743827 a.u.

C	1.30056400	-1.16670600	-0.00029400
H	0.97854900	-2.19937300	-0.00046300
C	2.59943400	-0.71944600	0.00071800
H	3.48141200	-1.34573900	0.00158100

C	1.30035700	1.16657400	-0.00087400
H	0.97816300	2.19918700	-0.00158500
C	2.59930800	0.71955300	0.00067400
H	3.48117300	1.34600500	0.00142000
C	0.43502500	-0.00015500	-0.00170500
Si	-1.28739100	-0.00004300	0.00008500
O	-2.28016600	1.29038100	0.00054100
H	-1.90890700	2.17726200	0.00121000
O	-2.28052600	-1.29019200	0.00019000
H	-1.90950400	-2.17717600	-0.00030800

I-F

E = -680.8793451 a.u.

C	1.29207000	-1.17596200	-0.00005400
H	0.95790500	-2.20286000	-0.00015700
C	2.58234600	-0.72368700	-0.00016800
H	3.46635400	-1.34674600	-0.00038200
C	1.29206400	1.17595900	0.00033000
H	0.95789300	2.20285500	0.00056400
C	2.58234200	0.72369100	0.00007500
H	3.46634700	1.34675500	0.00009100
C	0.43036900	-0.00000400	0.00025400
Si	-1.27545400	-0.00000200	-0.00009600
F	-2.22596600	-1.28155300	-0.00018700
F	-2.22595500	1.28155800	0.00003200

I-CF_3-T1

E = -1155.4993035 a.u.

C	2.32136200	-1.12989400	0.10147600
H	2.01363800	-2.16475000	0.17236400
C	3.67720200	-0.68283500	-0.17649500
H	4.51906500	-1.33508400	-0.35796600
C	2.32166100	1.12898900	0.10233400
H	2.01423700	2.16388400	0.17397800
C	3.67739500	0.68178900	-0.17598500
H	4.51944000	1.33393600	-0.35696500
C	1.47548600	-0.00042500	0.25065100
C	-1.18135300	1.57344200	-0.01328400
C	-1.18215000	-1.57309000	-0.01309200
Si	-0.28927000	-0.00001600	0.72956800
F	-2.47941200	1.65794300	0.35694100
F	-0.56772800	2.70771700	0.43779800
F	-1.15520900	1.63865100	-1.36725100
F	-2.47994900	-1.65741000	0.35846400
F	-0.56841400	-2.70760300	0.43685400
F	-1.15753600	-1.63770100	-1.36713800

I-SiH_3-T1

E = -1063.0233408 a.u.

C	1.83995900	1.12423800	0.04147000
H	1.53214900	2.16111700	0.09231200
C	3.21896400	0.68071900	-0.14449800
H	4.07175500	1.33385300	-0.26236100
C	1.83994600	-1.12427000	0.04142500
H	1.53212400	-2.16114700	0.09222000
C	3.21895600	-0.68075900	-0.14452500
H	4.07173900	-1.33389800	-0.26241400
C	0.98322700	-0.00001300	0.14687700
Si	-0.83466700	0.00000300	0.48146800
Si	-1.90152500	1.99002000	-0.15587000
H	-3.30224800	1.97347000	0.34220300
H	-1.20266500	3.15755000	0.44880700
H	-1.93754100	2.20203300	-1.63138400
Si	-1.90158800	-1.98999000	-0.15585200
H	-3.30233100	-1.97336400	0.34216400
H	-1.93755700	-2.20203400	-1.63136200
H	-1.20281400	-3.15754000	0.44888400

I-H-T1

E = -482.55997385 a.u.

C	0.57834000	-1.12419400	0.00272500
H	0.26295400	-2.16022700	-0.00127400
C	1.97065400	-0.68072100	0.00488100
H	2.83178200	-1.33352700	0.01209900
C	0.57833800	1.12418100	0.00274800
H	0.26288900	2.16019400	-0.00122900
C	1.97063700	0.68075700	0.00488200
H	2.83181400	1.33350100	0.01210000
C	-0.28207100	-0.00002600	0.01464900
Si	-2.12086100	-0.00000700	-0.08930000
H	-2.69643900	-1.22870400	0.52474100
H	-2.69633800	1.22888600	0.52444400

I-CN-T1

E = -666.6829261 a.u.

C	1.61069600	-1.13025200	-0.03982800
H	1.29700500	-2.16515600	-0.08765200
C	2.97769400	-0.68249100	0.17848200
H	3.82640000	-1.33449400	0.32491700
C	1.61109900	1.13022000	-0.04210100
H	1.29768000	2.16509200	-0.09182400
C	2.97789900	0.68232500	0.17735700
H	3.82674500	1.33443500	0.32272900

C	0.76405100	-0.00002100	-0.15777200
Si	-1.01554300	0.00021500	-0.54739400
C	-1.86441700	-1.50020100	0.09495100
C	-1.86448300	1.50017500	0.09588900
N	-2.37890800	-2.49768900	0.38165100
N	-2.37901300	2.49748700	0.38313200

I-Me-T1

E = -561.0113856 a.u.

C	1.30688800	-1.12180600	-0.04091800
H	0.99794700	-2.15911900	-0.08027500
C	2.69355900	-0.68008800	0.11205800
H	3.54854600	-1.33378000	0.21059100
C	1.30683500	1.12186800	-0.04073800
H	0.99789900	2.15919200	-0.07989900
C	2.69351000	0.68013900	0.11220400
H	3.54849300	1.33382200	0.21085800
C	0.44871400	0.00007900	-0.12496800
Si	-1.37983500	-0.00002800	-0.42897500
C	-2.19121300	-1.56644400	0.26537900
H	-1.74018100	-2.47047800	-0.15203900
H	-2.09045900	-1.61072500	1.35627100
H	-3.25711300	-1.58964300	0.02365500
C	-2.19143700	1.56634800	0.26520000
H	-2.09073900	1.61079400	1.35608800
H	-1.74051100	2.47038500	-0.15232800
H	-3.25733100	1.58937000	0.02342300

I-NH_2-T1

E = -593.1070668 a.u.

C	-1.38321000	-1.07144000	0.34414600
H	-1.16916300	-2.07918800	0.67999800
C	-2.72756900	-0.56129600	0.06604100
H	-3.64000300	-1.13581800	0.14164700
C	-1.18162500	1.08110200	-0.25998300
H	-0.76221300	2.05062000	-0.49658100
C	-2.60461300	0.74423300	-0.29761700
H	-3.39952600	1.42353600	-0.57112000
C	-0.43200100	-0.05407200	0.12270700
Si	1.40082200	-0.10836200	0.42699600
N	2.07811200	-1.32631600	-0.61847900
H	1.47423900	-1.97909300	-1.09854200
H	2.98416700	-1.73252300	-0.43386400
N	2.15898600	1.41371800	0.03489500
H	2.38657800	2.08149900	0.75685500
H	2.82883700	1.44504600	-0.72300300

I-Cl-T1

E = -1400.79882475 a.u.

C	1.73085300	-1.12784500	-0.05174200
H	1.41490300	-2.16198600	-0.09733600
C	3.10247500	-0.68160900	0.15827300
H	3.95200300	-1.33426600	0.29842200
C	1.73067300	1.12775600	-0.05203000
H	1.41465900	2.16186600	-0.09792400
C	3.10232500	0.68173200	0.15817500
H	3.95183300	1.33448900	0.29804500
C	0.88518500	-0.00002000	-0.16232400
Si	-0.90437000	0.00002100	-0.57885900
Cl	-1.80533200	-1.71448600	0.21759600
Cl	-1.80533200	1.71445700	0.21773900

I-OH-T1

E = -632.8355717 a.u.

C	-1.24234900	-1.12511600	0.04357700
H	-0.91932600	-2.15779700	0.06839100
C	-2.62750600	-0.68126400	-0.08836800
H	-3.48414300	-1.33393300	-0.17800600
C	-1.24219600	1.12517800	0.04384300
H	-0.91929600	2.15788700	0.06894700
C	-2.62753100	0.68126200	-0.08821300
H	-3.48417400	1.33395300	-0.17768000
C	-0.39310400	0.00009900	0.11111800
Si	1.42287400	0.00004000	0.38053600
O	1.99782600	-1.41055500	-0.32065100
H	2.85794200	-1.74278500	-0.05359000
O	1.99800800	1.41038100	-0.32099500
H	2.85820800	1.74255200	-0.05413300

I-F-T1

E = -680.854743 a.u.

C	1.23520700	-1.12682600	-0.04114000
H	0.91693600	-2.16095400	-0.07315000
C	2.61758600	-0.68227900	0.09756100
H	3.47229800	-1.33582600	0.19570800
C	1.23841100	1.12792200	-0.04696700
H	0.92311500	2.16280300	-0.08437200
C	2.61936900	0.68046600	0.09414300
H	3.47580300	1.33225400	0.18887900
C	0.38813600	0.00148400	-0.10653800
Si	-1.42454600	0.00183700	-0.40728300
F	-2.07803200	-1.31385500	0.30052300
F	-2.08160800	1.31067900	0.30975800

II-CF_3

E = -1155.5550719 a.u.

C	-2.44351400	-1.36711600	0.00737200
H	-2.30808300	-2.43810900	0.01483100
C	-3.64026000	-0.74773200	0.00437500
H	-4.58757500	-1.27810400	0.00801200
C	-2.44348000	1.36708000	-0.00759600
H	-2.30796400	2.43806300	-0.01515000
C	-3.64024500	0.74775200	-0.00391200
H	-4.58756000	1.27812900	-0.00701800
Si	-1.20302100	-0.00004300	-0.00034800
C	0.53011600	0.00005000	0.00009300
C	1.31128700	-1.27294600	-0.00016800
C	1.31130500	1.27298400	0.00019100
F	2.24347200	-1.32659300	0.97838500
F	1.97082400	-1.49559300	-1.16290900
F	0.49258200	-2.34780100	0.18213000
F	2.24345600	1.32662700	-0.97827800
F	0.49249600	2.34776600	-0.18216700
F	1.97075000	1.49561700	1.16306900

II-SiH_3

E = -1063.0774938 a.u.

C	1.85257200	1.36081000	-0.00008200
H	1.73271000	2.43479300	-0.00025000
C	3.05324300	0.74474900	0.00009800
H	4.00016800	1.27674200	0.00017900
C	1.85255900	-1.36083400	-0.00000600
H	1.73272300	-2.43482100	0.00010400
C	3.05323600	-0.74478000	0.00021100
H	4.00015600	-1.27678100	0.00048400
Si	0.59210300	-0.00000500	-0.00027900
C	-1.12545700	-0.00001000	-0.00008100
Si	-2.06540100	-1.60501600	0.00003300
H	-2.94283300	-1.71269700	1.19832000
H	-2.94280400	-1.71324000	-1.19824600
H	-1.13541300	-2.76685000	0.00006900
Si	-2.06533200	1.60504400	0.00010300
H	-2.94280800	1.71272100	1.19836900
H	-1.13530000	2.76684000	0.00033200
H	-2.94268900	1.71335600	-1.19819300

II-H

E = -482.6017485 a.u.

C	0.47870300	1.35976800	-0.00007300
H	0.36196800	2.43456000	-0.00012900
C	1.68175300	0.74265400	0.00009200
H	2.62805400	1.27578500	0.00017700
C	0.47869800	-1.35976800	-0.00007000
H	0.36196000	-2.43456000	-0.00010100
C	1.68175000	-0.74265800	0.00007900
H	2.62804900	-1.27579200	0.00018700
Si	-0.77475900	0.00000200	-0.00011400
C	-2.48755700	0.00000000	0.00015800
H	-3.06675100	0.91640300	0.00020100
H	-3.06674000	-0.91641000	0.00014700

II-CN

E = -666.6970707 a.u.

C	-1.62299500	-1.37255300	-0.00021200
H	-1.49222200	-2.44448400	-0.00043300
C	-2.81965600	-0.74755400	0.00012000
H	-3.76751500	-1.27656300	0.00021300
C	-1.62299300	1.37254400	0.00024700
H	-1.49221800	2.44447500	0.00041100
C	-2.81965500	0.74754700	0.00038200
H	-3.76751300	1.27655700	0.00069000
Si	-0.40074200	-0.00000500	-0.00018700
C	1.34832700	-0.00000200	-0.00006400
C	2.06501700	-1.22401300	-0.00019100
C	2.06499500	1.22402300	0.00008800
N	2.61227800	-2.24511300	-0.00028900
N	2.61223700	2.24513300	0.00022000

II-Me

E = -561.0307507 a.u.

C	-1.30675200	-1.35967900	0.00048500
H	-1.19734300	-2.43524100	0.00121100
C	-2.51349100	-0.73920800	0.00058000
H	-3.45841000	-1.27485600	0.00137300
C	-1.30773500	1.35985900	-0.00047300
H	-1.19931800	2.43551300	-0.00124700
C	-2.51397000	0.73835300	-0.00015700
H	-3.45920800	1.27344700	-0.00044300
Si	-0.06286800	0.00058300	-0.00050300
C	1.67090300	0.00001300	-0.00006700
C	2.47901600	-1.27218200	-0.00054000
H	3.13568400	-1.31485700	0.87903200
H	1.86303400	-2.17414300	-0.00025000
H	3.13451300	-1.31489400	-0.88096400
C	2.47965300	1.27186600	0.00090800
H	3.13616600	1.31485900	-0.87867500

H	1.86405700	2.17413700	0.00124000
H	3.13523400	1.31373200	0.88135200

II-NH_2

E = -593.0898431 a.u.

C	-1.19523500	1.19795100	0.44543100
H	-1.25250600	2.20578400	0.84708800
C	-2.22649700	0.68172100	-0.28252600
H	-3.12280500	1.24467500	-0.53734000
C	-0.98815700	-1.36711300	-0.26425000
H	-0.81041900	-2.40955400	-0.50794600
C	-2.10426100	-0.71648700	-0.68934300
H	-2.88618400	-1.18430900	-1.28400900
Si	-0.08634300	-0.24101700	0.96204500
C	1.52458300	0.08746400	-0.04034200
N	1.75485900	1.27453100	-0.61354200
H	0.98202500	1.92109200	-0.67003300
H	2.64889600	1.54898900	-1.00100300
N	2.51295000	-0.82146100	-0.10026600
H	3.32450700	-0.71631600	-0.69235500
H	2.38803100	-1.70883300	0.35979700

II-Cl

E = -1400.7272571 a.u.

C	-1.81776200	-1.36769300	-0.00018700
H	-1.69444500	-2.44051600	-0.00031700
C	-3.01979600	-0.74111600	0.00021200
H	-3.96573300	-1.27391800	0.00040800
C	-1.81776100	1.36769000	-0.00010900
H	-1.69444400	2.44051300	-0.00015800
C	-3.01979500	0.74111300	0.00024300
H	-3.96573300	1.27391500	0.00049000
Si	-0.59531900	-0.00000200	-0.00029400
C	1.14157200	-0.00000400	0.00006700
Cl	2.08399600	1.47074200	0.00004300
Cl	2.08400800	-1.47073700	0.00009400

II-OH

E = -632.7725129 a.u.

C	-1.11387100	1.31469500	0.17273300
H	-1.04682000	2.38214600	0.35393400
C	-2.24368200	0.75828500	-0.34587400
H	-3.10900500	1.34302700	-0.64841700
C	-1.18087900	-1.37467500	-0.01789900
H	-1.09653300	-2.45285600	-0.05731700
C	-2.27301700	-0.70098200	-0.46431600
H	-3.14240100	-1.19363500	-0.89226000
Si	-0.07880600	-0.11282600	0.80200900
C	1.55313300	-0.02041100	-0.06170600
O	2.17522900	1.12686200	-0.37359000
H	1.52462800	1.84346700	-0.38730000
O	2.36215300	-1.05745200	-0.21930000
H	3.22426300	-0.75933200	-0.55126900

II-F

E = -680.7435279 a.u.

C	0.00776300	1.25555900	1.36889200
H	-0.00644900	1.13603200	2.44198100
C	0.12758100	2.45271300	0.73829500
H	0.22528600	3.39255400	1.27277500
C	0.00776300	1.25555900	-1.36889200
H	-0.00644900	1.13603200	-2.44198100
C	0.12758100	2.45271300	-0.73829500
H	0.22528600	3.39255400	-1.27277500
Si	-0.15866600	0.05375100	0.00000000
C	0.00330000	-1.68591200	0.00000000
F	0.00776300	-2.45519300	1.08989200
F	0.00776300	-2.45519300	-1.08989200

II-CF_3-T1

E = -1155.4930517 a.u.

C	-2.38195200	-0.26190000	1.36670300
H	-2.27303300	-0.23218900	2.44153200
C	-3.55148600	-0.02833500	0.71846100
H	-4.47615700	0.21420200	1.23426300
C	-2.35998700	-0.43734400	-1.34807100
H	-2.23146800	-0.54554800	-2.41566100
C	-3.53962500	-0.12441700	-0.75485600
H	-4.45570500	0.04760400	-1.31262500
Si	-1.19728000	-0.77876100	0.04757100
C	0.55580900	-0.08930900	0.03199500
C	1.74519400	-1.00826300	0.02380300
C	0.83560000	1.38765500	-0.02338600
F	2.86000400	-0.45370400	0.53070600
F	2.03325300	-1.41132800	-1.23838200
F	1.49158200	-2.12684700	0.74311600
F	1.74542700	1.70221200	-0.97097700
F	-0.28530200	2.08477000	-0.29974900
F	1.30803100	1.84823700	1.15735300

II-SiH_3-T1

E = -1063.0162384 a.u.

C	1.82147300	-0.18075900	-1.35460000
H	1.70705600	-0.22025900	-2.42900100

C	3.01698900	0.03135000	-0.73438100
H	3.94746100	0.17887400	-1.27543600
C	1.82145100	-0.18096200	1.35458600
H	1.70701600	-0.22062200	2.42898000
C	3.01697700	0.03123900	0.73441800
H	3.94744100	0.17868200	1.27551000
Si	-1.57913500	1.81355600	0.00006300
H	-2.39675500	2.13033300	1.20404900
H	-0.36293600	2.66257200	0.00014700
H	-2.39666300	2.13044100	-1.20395700
Si	-2.51796600	-1.28373200	-0.00003700
H	-3.85212000	-0.62791200	-0.00008900
H	-2.40638100	-2.15041900	-1.20464300
H	-2.40644900	-2.15035800	1.20461900
Si	0.62271800	-0.53399000	-0.00004300
C	-1.15127300	-0.00970200	-0.00001200

II-H-T1

E = -482.5473984 a.u.

C	0.46755200	1.35356600	0.01810100
H	0.35009200	2.42793500	0.04868700
C	1.67560900	0.73464800	-0.11620300
H	2.61299000	1.27605000	-0.20716100
C	0.46755200	-1.35356600	0.01806300
H	0.35010500	-2.42793600	0.04869600
C	1.67561300	-0.73464400	-0.11619800
H	2.61300400	-1.27604400	-0.20706800
Si	-0.74928400	-0.00000500	0.28564600
C	-2.50547600	0.00000800	-0.26717500
H	-2.77531700	0.00006100	-1.32093700
H	-3.34600100	-0.00007600	0.41921500

II-CN-T1

E = -666.5911189 a.u.

C	1.89960100	1.36422500	-0.00008300
H	1.77410400	2.43477200	-0.00126300
C	3.10379200	0.74608900	0.00030300
H	4.04672800	1.27942600	0.00039900
C	1.89961200	-1.36418300	-0.00032700
H	1.77413300	-2.43473200	0.00054800
C	3.10379400	-0.74602800	0.00057500
H	4.04673000	-1.27936500	0.00145500
Si	0.59806400	0.00001700	-0.00068800
C	-1.13655100	0.00004200	-0.00008300
C	-1.92814686	1.32101737	0.00018618
C	-1.92800774	-1.32101674	0.00004709
N	-2.51752595	2.30454358	0.00038659
N	-2.51728326	-2.30460503	0.00014394

II-Me-T1

E = -560.9813804 a.u.

C	-1.29908400	-1.35254700	-0.06064400
H	-1.18565200	-2.42779200	-0.08774400
C	-2.49845400	-0.73353900	0.13532200
H	-3.42952600	-1.27316700	0.28477000
C	-1.29924800	1.35055900	-0.09028600
H	-1.18576200	2.42497900	-0.14020600
C	-2.49850100	0.73588200	0.11946300
H	-3.42952800	1.27855400	0.25773000
Si	-0.09200600	-0.00459200	-0.41061700
C	1.70431300	0.00091100	0.02881300
C	2.80392600	-0.01436000	-0.99295900
H	3.45359600	-0.89139700	-0.85587100
H	2.43725200	-0.02841200	-2.02095500
H	3.45540100	0.86487600	-0.88058000
C	2.14217200	0.02000500	1.46825500
H	1.30987600	0.03012300	2.17426600
H	2.76527800	-0.85722000	1.69659700
H	2.76640700	0.90227800	1.67284600

II-NH_2-T1

E = -593.0367691 a.u.

C	-1.26980300	1.21293100	0.55609100
H	-1.15422200	2.19770100	0.98891700
C	-2.46623900	0.72987500	0.12060500
H	-3.39167000	1.29745800	0.16437700
C	-1.28520100	-1.30196000	-0.43220300
H	-1.17547600	-2.31768300	-0.78780300
C	-2.47441100	-0.64198400	-0.41601300
H	-3.40603300	-1.07892400	-0.76555900
Si	-0.06682900	-0.17716700	0.40040200
C	1.71747200	0.09204400	0.02820500
N	2.17222000	0.84614500	-1.07418200
H	2.64509900	0.30150700	-1.79424000
H	1.47732400	1.45498500	-1.48294600
N	2.75414700	-0.65157700	0.61075800
H	2.50657300	-1.15313400	1.45239500
H	3.61854300	-0.12897500	0.72308900

II-Cl-T1

E = -1400.6875312 a.u.

C	-1.78589600	0.16445600	-1.35844500
H	-1.66946900	0.20575700	-2.43232200

C	-2.96389800	-0.10054100	-0.73912600
H	-3.88648500	-0.30228400	-1.27599200
C	-1.78591000	0.16403000	1.35847500
H	-1.66949000	0.20499800	2.43236600
C	-2.96390500	-0.10077400	0.73906100
H	-3.88649200	-0.30270100	1.27585900
Si	-0.60532400	0.58468500	0.00008600
C	1.16559800	0.02383000	0.00006300
Cl	2.49437500	1.13620800	0.00008300
Cl	1.59918500	-1.65958200	-0.00015800

II-OH-T1

E = -632.7251268 a.u.

C	-1.25540900	-1.33951200	-0.32286900
H	-1.14066700	-2.37874800	-0.59887800
C	-2.43071000	-0.66560200	-0.41269700
H	-3.35062800	-1.11467300	-0.77736100
C	-1.24870200	1.24712300	0.47739000
H	-1.14368500	2.25837700	0.84716600
C	-2.42838600	0.74415000	0.02277300
H	-3.34710600	1.32236200	-0.02098300
Si	-0.06448000	-0.16761600	0.48987800
C	1.71508900	0.15395600	0.06187200
O	2.14056100	0.63420900	-1.16436100
H	1.54978100	1.33723700	-1.45823400
O	2.69419700	-0.58462000	0.65322700
H	3.54566400	-0.31532600	0.28025800

II-F-T1

E = -680.7040222 a.u.

C	1.88408326	1.35728737	-0.02476551
H	1.77289994	2.42650795	-0.13741620
C	3.05592743	0.69842251	-0.20160288
H	3.98008181	1.19445693	-0.48468372
C	1.86973698	-1.33278262	0.37130826
H	1.74825617	-2.38931280	0.56449564
C	3.04838670	-0.76576211	0.01099023
H	3.96518378	-1.33199894	-0.12484084
Si	0.69748342	0.07320920	0.58924149
C	-1.07582018	-0.12200994	0.02504422
F	-2.09301631	0.45221700	0.68174151
F	-1.40403758	-0.25996063	-1.26849219

III-CF_3

E = -1156.7079464 a.u.

Si	-0.17418400	0.02536500	-0.45886200
C	1.55924700	0.00152600	-0.08792500
C	2.28153300	1.27494000	-0.01997500
H	1.70683700	2.13783000	0.30227500
C	2.24389800	-1.28936400	-0.05320200
H	1.69841700	-2.13597700	-0.45762000
C	3.56290900	1.48114100	-0.36280300
H	3.99776200	2.47018100	-0.27862300
H	4.19550300	0.69653900	-0.75745500
C	3.42762300	-1.54851400	0.52841400
H	4.02231000	-0.78688600	1.01487200
H	3.79976400	-2.56523400	0.56875700
C	-1.22791200	-1.56779000	-0.06931400
C	-1.21646700	1.58344800	0.07101600
F	-0.65591300	-2.68227000	-0.59808700
F	-1.38698500	-1.80461500	1.25483700
F	-2.46989800	-1.47371700	-0.59938100
F	-2.40765100	1.62882200	-0.56899000
F	-0.56502100	2.73923200	-0.22158500
F	-1.48864500	1.61656000	1.39927300

III-SiH_3

E = -1064.2443831 a.u.

Si	0.75962600	-0.00000600	-0.00000900
C	-1.01332300	-0.00004200	-0.00008200
C	-1.71256000	-1.28562300	0.00003300
H	-1.11533800	-2.14072600	0.31036500
C	-1.71255900	1.28555900	-0.00022900
H	-1.11542700	2.14060000	-0.31091500
C	-2.97097200	-1.54759900	-0.39156800
H	-3.34456800	-2.56488500	-0.37780700
H	-3.64053700	-0.78455100	-0.76544600
C	-2.97083900	1.54759800	0.39173100
H	-3.64025700	0.78460500	0.76598500
H	-3.34445700	2.56487600	0.37791200
Si	1.94720400	2.01927600	-0.12522000
H	1.21098000	3.01307100	-0.94932300
H	2.18443500	2.60440600	1.22107200
H	3.26644500	1.74895700	-0.75464400
Si	1.94731200	-2.01922800	0.12525800
H	1.21040300	-3.01352200	0.94814000
H	2.18589200	-2.60364800	-1.22110700
H	3.26594700	-1.74913200	0.75604900

III-H

E = -483.7801739 a.u.

Si	-1.98122400	0.00002700	-0.00001400
C	-0.23102700	0.00002100	-0.00001100

C	0.44806600	-1.29058500	0.13117500
H	-0.18447500	-2.10892300	0.47219600
C	0.44812900	1.29062300	-0.13108200
H	-0.18443100	2.10907700	-0.47179100
C	1.71938000	-1.60473800	-0.16683900
H	2.06600900	-2.62538400	-0.05446800
H	2.42894600	-0.88887200	-0.55799200
C	1.71950600	1.60464300	0.16677800
H	2.42909500	0.88868000	0.55771200
H	2.06617900	2.62529300	0.05455300
H	-2.75421000	-1.24208000	0.18843000
H	-2.75430200	1.24205600	-0.18857100

III-CN

E = -667.8943524 a.u.

Si	0.92096600	-0.00000800	-0.00005800
C	-0.82783200	0.00001300	-0.00001400
C	-1.50563600	-1.29501800	0.03587400
H	-0.90170600	-2.13737200	0.36558600
C	-1.50559200	1.29503700	-0.03571300
H	-0.90157000	2.13746700	-0.36507500
C	-2.76171400	-1.56192600	-0.35578600
H	-3.13743800	-2.57726000	-0.31701300
H	-3.42673300	-0.80647700	-0.75214200
C	-2.76176400	1.56190100	0.35570700
H	-3.42689200	0.80638900	0.75176000
H	-3.13744100	2.57725500	0.31707000
C	1.90877200	1.51668400	-0.09494900
C	1.90878700	-1.51667900	0.09499800
N	2.52199900	2.49693400	-0.16215300
N	2.52202000	-2.49692800	0.16214400

III-Me

E = -562.2324365 a.u.

Si	1.25210300	0.00000100	-0.00001200
C	-0.50057000	0.00000700	0.00004400
C	-1.18977200	-1.29121000	0.05938400
H	-0.56495400	-2.13391600	0.34997600
C	-1.18976800	1.29122200	-0.05927100
H	-0.56490400	2.13396600	-0.34964900
C	-2.46672600	-1.59099500	-0.23461300
H	-2.80920200	-2.61745800	-0.17118900
H	-3.18510600	-0.85822600	-0.57409500
C	-2.46677700	1.59097500	0.23453200
H	-3.18522400	0.85817200	0.57379600
H	-2.80923200	2.61744900	0.17117200
C	2.28427100	1.56180200	-0.12806300
H	1.67158800	2.44334100	-0.32096500
H	2.84043700	1.73524500	0.79856700
H	3.01780400	1.47117300	-0.93490400
C	2.28426500	-1.56180000	0.12802900
H	3.01778800	-1.47115500	0.93487900
H	1.67157000	-2.44333100	0.32092800
H	2.84044900	-1.73526300	-0.79858800

III-NH_2

E = -594.3292182 a.u.

Si	1.25318800	0.00000600	0.00002300
C	-0.48834100	0.00002000	0.00003600
C	-1.15029900	-1.29048700	0.17402700
H	-0.49233100	-2.10046200	0.49208700
C	-1.15026500	1.29055800	-0.17388600
H	-0.49222000	2.10059700	-0.49161500
C	-2.43861100	-1.63451200	-0.01053100
H	-2.75151000	-2.65911200	0.15379700
H	-3.19651900	-0.94297600	-0.34848200
C	-2.43862700	1.63453100	0.01042900
H	-3.19660000	0.94288900	0.34802100
H	-2.75150800	2.65916300	-0.15372100
N	2.23369700	1.37950200	0.15790100
H	1.89412800	2.24142600	0.55597700
H	3.13718700	1.47462400	-0.28053300
N	2.23356800	-1.37957600	-0.15802900
H	1.89370600	-2.24152200	-0.55581400
H	3.13704000	-1.47484300	0.28041600

III-Cl

E = -1402.0053795 a.u.

Si	0.76797100	-0.00006100	-0.00089000
C	-0.96939200	-0.00002300	0.00008800
C	-1.63749700	-1.30274700	0.04474000
H	-1.01086200	-2.14102400	0.34059500
C	-1.63748900	1.30271700	-0.04465700
H	-1.01084500	2.14097200	-0.34053600
C	-2.90959700	-1.59148800	-0.27159900
H	-3.25887500	-2.61552200	-0.21478900
H	-3.61747100	-0.85104700	-0.61658000
C	-2.90952900	1.59153300	0.27185500
H	-3.61746100	0.85112900	0.61679200
H	-3.25868000	2.61562300	0.21527800
Cl	1.92361500	1.68270400	-0.09074500
Cl	1.92365700	-1.68265800	0.09128200

III-OH

E = -634.0422368 a.u.

Si	-1.25592800	0.00002500	-0.00051700
C	0.47348600	0.00000500	0.00026400
C	1.12423600	-1.30824200	-0.07790600
H	0.45273000	-2.13668000	-0.29719800
C	1.12412500	1.30834000	0.07795900
H	0.45251200	2.13675600	0.29704100
C	2.41434000	-1.63184600	0.11429000
H	2.72337100	-2.66791700	0.03983500
H	3.17850600	-0.91531000	0.37648500
C	2.41420800	1.63202700	-0.11420100
H	3.17845900	0.91548900	-0.37615400
H	2.72315700	2.66813200	-0.03989300
O	-2.15622100	-1.37475900	0.03489700
H	-2.96227000	-1.46365000	-0.48026600
O	-2.15699300	1.37430600	-0.03485200
H	-2.96012500	1.46475400	0.48458500

III-F

E = -682.0551173 a.u.

Si	-1.26910600	-0.00875100	0.15120200
C	0.45674700	0.00403900	-0.05947800
F	-2.19394700	-1.27675200	-0.18975000
F	-2.19872800	1.29584800	0.03241000
C	1.10154900	-1.31055500	-0.09775200
H	0.45885600	-2.13208000	-0.41034100
C	1.11607600	1.30428900	0.05250600
H	0.45877100	2.13800200	0.29084000
C	2.37518300	-1.61856900	0.19252000
H	2.72190300	-2.63948600	0.08575500
H	3.09137800	-0.89443400	0.55425300
C	2.40122000	1.61226900	-0.18799400
H	3.14518200	0.88330600	-0.47455200
H	2.72081300	2.64651500	-0.14553200

IV-CF_3

E = -1156.7491868 a.u.

C	2.20518400	1.56505200	0.12319700
H	1.71548100	2.42430500	0.57069600
C	2.20556200	-1.56333600	-0.12612300
H	1.71783900	-2.42086400	-0.57912300
C	3.45198400	1.70696300	-0.34457900
H	3.97705000	2.65454200	-0.26802400
H	3.99111500	0.90282100	-0.83432000
C	3.44992800	-1.70746700	0.34734300
H	3.98696100	-0.90535300	0.84269700
H	3.97500100	-2.65498200	0.27005200
C	-0.50969400	0.00021000	-0.00018400
Si	1.23178200	0.00075500	-0.00100700
C	-1.31227700	-1.25797100	-0.03849100
C	-1.31341700	1.25758700	0.03876000
F	-1.83320600	-1.53107600	-1.26558100
F	-0.56255400	-2.34896500	0.29072300
F	-2.36151400	-1.24401500	0.81618000
F	-0.56494200	2.34924300	-0.29115200
F	-2.36341200	1.24262200	-0.81504000
F	-1.83348700	1.53027300	1.26626800

IV-SiH_3

E = -1064.2682173 a.u.

C	1.63118300	-1.56126700	-0.10375800
H	1.13378300	-2.43057000	-0.52733500
C	1.63118900	1.56130500	0.10380500
H	1.13384400	2.43062000	0.52741800
C	2.88358300	-1.71344800	0.34608700
H	3.39688400	-2.66893200	0.28338500
H	3.44141200	-0.90442400	0.80651200
C	2.88356700	1.71344000	-0.34612000
H	3.44132700	0.90440200	-0.80660400
H	3.39691100	2.66890300	-0.28344700
C	-1.08961900	0.00000300	0.00000000
Si	0.63296900	0.00002100	0.00001400
Si	-2.07778100	1.57006400	0.09786900
H	-1.22359300	2.75283900	0.39435800
H	-2.79777500	1.84858200	-1.17669000
H	-3.11268900	1.48160400	1.16640000
Si	-2.07773300	-1.57009100	-0.09787900
H	-1.22353100	-2.75282600	-0.39448200
H	-2.79765800	-1.84864700	1.17670900
H	-3.11270700	-1.48165800	-1.16634900

IV-H

E = -483.7926691 a.u.

C	0.26761900	-1.59059200	-0.14431100
H	-0.31532200	-2.43933400	-0.50056400
C	0.26944500	1.58994900	0.14543300
H	-0.31197800	2.43854500	0.50450800
C	1.55018800	-1.80575200	0.17514700
H	2.00301500	-2.78851500	0.08000200
H	2.19609400	-1.02220100	0.55726500
C	1.55170200	1.80447700	-0.17567000

H	2.19614400	1.02113200	-0.56068100
H	2.00570700	2.78656900	-0.07920400
H	-2.96633000	-0.90823800	-0.09372600
H	-2.96517100	0.91170700	0.09268600
C	-2.38349300	0.00131000	-0.00029000
Si	-0.66963800	0.00028400	-0.00015300

IV-CN

E = -667.8948153 a.u.

C	1.33422200	1.60878700	0.08258800
H	0.74124900	2.45983500	0.41142800
C	1.33405100	-1.60897500	-0.08100300
H	0.74018900	-2.46044900	-0.40714700
C	2.61076400	1.80941400	-0.27200100
H	3.06031000	2.79646800	-0.22338200
H	3.25138000	1.01389500	-0.63797100
C	2.61147600	-1.80915800	0.27065900
H	3.25307200	-1.01311200	0.63375800
H	3.06081300	-2.79632300	0.22240900
C	-1.30200200	-0.00002800	-0.00003600
Si	0.45217500	-0.00005800	0.00045700
C	-2.01791000	-1.22196100	-0.06520100
C	-2.01783800	1.22196600	0.06472700
N	-2.55391700	-2.24799600	-0.12359000
N	-2.55380300	2.24802800	0.12303300

IV-Me

E = -562.2198132 a.u.

C	-1.05950100	1.59124700	0.11124700
H	-0.49592400	2.45347200	0.46435100
C	-1.05937100	-1.59080500	-0.10901500
H	-0.49359600	-2.45318100	-0.45834100
C	-2.34558100	1.79015100	-0.20999900
H	-2.80884800	2.76853200	-0.12003600
H	-2.98288500	0.99728000	-0.58708300
C	-2.34641100	-1.79047500	0.20784100
H	-2.98597900	-0.99758000	0.58103000
H	-2.80822000	-2.76955000	0.11804600
C	1.61677100	-0.00018400	-0.00037400
Si	-0.11685000	0.00020100	0.00106300
C	2.44141600	-1.26235600	-0.07763600
H	3.08582400	-1.36075600	0.80713000
H	1.84309500	-2.17326300	-0.14585100
H	3.11163100	-1.23826100	-0.94802700
C	2.44118100	1.26220700	0.07648300
H	3.08502100	1.36042800	-0.80869800
H	1.84276800	2.17300900	0.14482400
H	3.11199300	1.23834500	0.94648700

IV-NH_2

E = -594.2692752 a.u.

C	-0.84695500	1.60616900	-0.29752000
H	-0.38780100	2.46215400	-0.80179300
C	-1.00750200	-1.45191000	0.22482600
H	-0.35240600	-2.11262300	0.79963800
C	-1.92388800	1.87593400	0.45340900
H	-2.30316500	2.88784800	0.57702700
H	-2.47536300	1.09254800	0.96510100
C	-2.31614700	-1.74095500	0.26608100
H	-3.05569900	-1.16471000	-0.28329700
H	-2.70514800	-2.56965600	0.85223700
C	1.54262100	-0.05800500	0.03288000
Si	-0.16758500	-0.09813400	-0.80333800
N	2.31762000	-1.16226300	0.09377000
H	1.97327200	-2.03018000	-0.28285100
H	3.23003100	-1.17112600	0.52475800
N	2.12024100	1.08764900	0.44409700
H	1.54738200	1.91303300	0.51915300
H	3.12129000	1.20148000	0.53362400

IV-Cl

E = -1401.9201148 a.u.

C	1.52172900	1.61590900	0.07939800
H	0.91150100	2.46641000	0.37568600
C	1.52178800	-1.61570900	-0.07923100
H	0.91131400	-2.46609000	-0.37538200
C	2.81328700	1.82894400	-0.20720300
H	3.24967300	2.82090100	-0.14024300
H	3.48154600	1.03828300	-0.53115500
C	2.81340800	-1.82900800	0.20687800
H	3.48193300	-1.03851000	0.53068500
H	3.24958700	-2.82103400	0.13961600
C	-1.09528500	-0.00001700	-0.00002900
Si	0.64192100	0.00006800	0.00028700
Cl	-2.05060200	-1.46963500	-0.06102200
Cl	-2.05069300	1.46953900	0.06089900

IV-OH

E = -633.9538250 a.u.

C	0.97719500	-1.63937200	-0.03632700
H	0.28583100	-2.47942500	-0.08670700
C	0.97739100	1.63959600	0.03614400
H	0.28640300	2.47996400	0.08617500

C	2.29063700	-1.90740000	-0.00174300
H	2.65903800	-2.92844500	-0.02763300
H	3.04899500	-1.13462200	0.05658200
C	2.29098700	1.90696200	0.00204100
H	3.04896400	1.13378500	-0.05592400
H	2.65991100	2.92781800	0.02799700
O	-2.35005400	-1.14694100	0.13961500
H	-3.01050700	-1.17755900	-0.56872400
O	-2.35025600	1.14690400	-0.13941200
H	-3.01040500	1.17758500	0.56920700
C	-1.60238400	0.00003400	0.00004700
Si	0.14509200	0.00016200	-0.00025500

IV-F

E = -681.9346944 a.u.

F	-2.37501900	-1.09334100	0.00157700
F	-2.37546600	1.09324300	0.00220100
C	0.94897400	-1.65022100	-0.00120200
H	0.25240600	-2.48720000	-0.00418200
C	0.94935200	1.65039500	0.00052000
H	0.25335700	2.48784700	0.00325700
C	2.26122700	-1.92143200	0.00382700
H	2.62383600	-2.94449600	0.00561200
H	3.02400900	-1.15094800	0.00678500
C	2.26181100	1.92076500	0.00125500
H	3.02407200	1.14976500	-0.00186700
H	2.62510900	2.94357600	0.00492100
C	-1.59843000	0.00011600	0.00151200
Si	0.14385500	0.00032900	-0.00600000

V-CF_3

E = -1266.0006493 a.u.

C	0.44697035	1.14941727	0.00051237
C	1.19614115	0.01628337	0.00256702
C	-0.97993054	-0.74879150	-0.00102646
C	0.31674956	-1.15355911	-0.00102646
C	-0.97993054	0.73664997	-0.00102646
H	2.27705275	-0.02211354	0.03619585
H	0.65404101	-2.18126363	-0.03316305
N	0.86628098	2.48188160	0.17035553
H	1.85706811	2.55097588	0.36321978
H	0.62601861	3.10111623	-0.59468248
N	-2.14329287	-1.52190433	-0.17143076
H	-1.93430765	-2.49314905	-0.36279911
H	-2.80591069	-1.46204658	0.59263849
Si	-2.35946750	1.77366125	-0.00250737
C	-4.21120225	1.22069991	0.24438960
C	-2.34221053	3.70592323	-0.25126338
F	-4.31418609	0.13062818	1.04624950
F	-4.91180125	2.21059255	0.84679807
F	-4.84476331	0.92771989	-0.90868721
F	-2.23738345	4.39702085	0.90116695
F	-3.48689432	4.10389455	-0.85509617
F	-1.32262821	4.10638481	-1.05271331

V-SiH_3

E = -1173.5440254 a.u.

C	-0.97599053	-0.73276583	0.00528941
C	0.32006035	-1.15462992	0.04847699
C	0.43286642	1.13930680	-0.06434523
C	1.19905429	0.01338870	0.00528941
C	-0.97599053	0.73470025	0.00528941
H	0.65593972	-2.18314646	0.08910722
H	2.28115012	-0.02355275	0.00922364
N	-2.18102151	-1.48611102	0.04743481
H	-2.64133652	-1.53330472	-0.85682223
H	-2.02252937	-2.43329265	0.37103557
N	0.82325944	2.50593063	-0.10106399
H	1.78809444	2.63029274	0.18286754
H	0.70872626	2.91793438	-1.02244143
Si	-2.33170238	1.76941617	0.39483322
Si	-4.44150622	0.80156507	0.78314375
H	-4.92377121	0.03921265	-0.39590170
H	-4.41109881	-0.06589018	1.98489225
H	-5.40110722	1.91480807	1.02703145
Si	-1.97426510	4.08031892	0.66084762
H	-1.08983250	4.34756563	1.82014584
H	-1.41864453	4.69747651	-0.56972197
H	-3.30061328	4.70612082	0.92312552

V-H

E = -593.0766145 a.u.

C	1.22126855	0.06597560	-0.06381992
C	0.38137954	1.13615630	-0.02813189
C	-1.00201894	-0.70352060	0.03065060
C	-1.00201894	0.65735187	0.03065060
C	0.40138977	-1.15596318	0.03065060
H	0.67615654	2.17721804	-0.06130198
H	-1.87790533	1.29323838	0.04722360
N	2.63527485	0.03680451	-0.07735002
H	3.01706812	-0.43570890	-0.88990086
H	3.03496079	0.96529583	-0.02111321

N	-2.09245288	-1.59949695	0.12353761
H	-2.97425185	-1.11453701	0.23422646
H	-2.16140895	-2.22801804	-0.66986027
Si	0.96908546	-2.75213452	0.38952372
H	0.05387536	-3.89235464	0.57376529
H	2.40352277	-3.07912433	0.47392555

V-CN

E = -777.1877997 a.u.

C	0.05142900	1.50188800	1.18551800
C	-0.10457700	2.77382700	0.73483900
C	0.05142900	1.50188800	-1.18551800
C	-0.10457700	2.77382700	-0.73483900
C	0.10271400	0.62053700	0.00000000
H	-0.19496900	3.65746900	1.35243400
H	-0.19496900	3.65746900	-1.35243400
N	0.03978800	0.99999900	2.50015300
H	0.88292800	0.50424200	2.76797000
H	-0.16576800	1.71139100	3.18961800
N	0.03978800	0.99999900	-2.50015300
H	-0.16576800	1.71139100	-3.18961800
H	0.88292800	0.50424200	-2.76797000
C	-0.04238900	-2.14109600	1.48812400
C	-0.04238900	-2.14109600	-1.48812400
N	-0.01859200	-2.83692700	2.41234100
N	-0.01859200	-2.83692700	-2.41234100
Si	-0.05792600	-1.09770400	0.00000000

V-Me

E = -671.5340995a.u.

C	0.43721132	1.13475041	0.06557684
C	1.19803388	0.00101141	0.02862109
C	-0.97736099	-0.72587420	-0.03139931
C	0.31947679	-1.15458290	-0.03139931
C	-0.97736099	0.74469527	-0.03139931
H	2.27942240	-0.03777135	0.07090495
H	0.64521041	-2.18729961	-0.04077442
N	0.87778884	2.48853611	0.11429975
H	0.66731854	2.92765357	1.00613148
H	1.87906015	2.54813336	-0.03154691
N	-2.16366027	-1.51197809	-0.09423384
H	-1.94463853	-2.48133713	-0.29358096
H	-2.68738315	-1.48471020	0.77608469
Si	-2.30827654	1.77922969	-0.46623972
C	-4.02993139	1.12686623	-0.79037073
H	-3.98104234	0.05249532	-0.97494835
H	-4.68845337	1.30472900	0.06635336
H	-4.47563445	1.63057732	-1.65313176
C	-2.12702310	3.62973711	-0.65990222
H	-2.51798242	4.15950758	0.21517233
H	-1.07116331	3.87982499	-0.77544013
H	-2.68803751	3.98179034	-1.53056443

V-NH_2

E = -703.6444789 a.u.

C	-0.35062120	1.15969580	0.03588140
C	0.95218880	0.71874880	-0.09051460
C	-0.35058420	-1.15970220	0.03598740
C	0.95221480	-0.71872320	-0.09044760
C	-1.20319820	-0.00001920	0.10909340
H	1.83020180	1.34842980	-0.16610560
H	1.83024780	-1.34838520	-0.16594860
N	-0.86862420	2.50771780	0.08266240
H	-0.68831120	2.93626780	0.98708340
H	-0.41293220	3.09214880	-0.61138060
N	-0.86851820	-2.50773120	0.08284440
H	-0.41193520	-3.09247120	-0.61034560
H	-0.68926820	-2.93580120	0.98770940
Si	-2.93830420	-0.00003620	0.01067240
N	-3.83193120	-1.42581120	-0.03966060
H	-4.82914520	-1.53401220	-0.12506560
H	-3.28973020	-2.28476120	-0.05199560
N	-3.83205220	1.42567780	-0.03896560
H	-3.28988720	2.28465580	-0.05104260
H	-4.82919720	1.53380680	-0.12528260

V-Cl

E = -1511.3039493 a.u.

C	0.43734884	1.14749107	0.04410355
C	1.19495019	0.01575588	0.01911151
C	-0.97747597	-0.74434642	-0.02107168
C	0.32265291	-1.15063918	-0.02107168
C	-0.97747597	0.73173865	-0.02107168
H	2.27625263	-0.01650772	0.05089147
H	0.65873132	-2.17938147	-0.02362117
N	0.86031519	2.49517158	0.01989752
H	0.54522808	3.03740448	0.81747643
H	1.86754942	2.56944953	-0.04882769
N	-2.14865035	-1.52827621	-0.11871331
H	-1.93234767	-2.51159491	-0.22387355
H	-2.78394279	-1.41420689	0.66411503
Si	-2.32980367	1.75338927	-0.32011370

Cl	-4.26065710	1.13071838	-0.51155849
Cl	-2.27343212	3.78794255	-0.42001509

V-OH

E = -743.3623086 a.u.

C	0.08424660	-1.21563160	0.01822760
C	-1.08536440	-0.49301360	-0.06075440
C	0.58801060	1.06682940	0.02699060
C	-0.76976640	0.91580140	-0.05647040
C	1.18287360	-0.27398560	0.07200660
H	-2.08188640	-0.91105160	-0.11807840
H	-1.49491140	1.71895340	-0.09638640
N	0.24480860	-2.61433260	-0.04575040
H	0.89948360	-2.98600760	0.63155660
H	-0.63415040	-3.11019060	0.02375760
N	1.38462760	2.27837340	0.07312560
H	1.12792660	2.90980640	-0.68026440
H	1.23933360	2.78466540	0.94346560
Si	2.89723660	-0.40145660	-0.01613440
O	3.78547060	-1.76629160	0.00130160
H	4.74352560	-1.71736360	-0.07078040
O	3.80406960	0.94459940	-0.07054140
H	3.15790360	1.70850040	-0.04938340

V-F

E = -791.3558060 a.u.

C	-0.97579008	-0.74681501	0.01308912
C	0.32763373	-1.14852459	0.01308912
C	0.42978379	1.15091509	-0.02739701
C	1.19416263	0.02141601	-0.01187036
C	-0.97579008	0.72300849	0.01308912
H	0.66810162	-2.17576399	0.00468551
H	2.27564717	-0.00534261	-0.04161822
N	-2.16139091	-1.51420555	0.09286650
H	-2.74618863	-1.44164028	-0.73351827
H	-1.96821805	-2.49180286	0.27084861
N	0.81939919	2.51029663	0.00700783
H	1.81424592	2.61507617	0.16189852
H	0.56255193	3.02564293	-0.82882323
Si	-2.29863158	1.71200458	0.44524217
F	-2.30885839	3.30276455	0.57719631
F	-3.82014676	1.26230444	0.62072746

V-CF_3-T0

E = -1266.0104828 a.u.

C	0.41336005	1.12341808	-0.00133903
C	1.20605725	-0.06565216	-0.00114361
C	-0.98733475	-0.67374138	0.00082755
C	0.35525219	-1.15621267	0.00082755
C	-0.98733475	0.77218814	0.00082755
H	2.28650467	-0.08841212	0.03172430
H	0.64013539	-2.19878443	0.02574010
N	0.95172315	2.37067508	0.00285159
H	0.40547441	3.16998399	0.28318591
H	1.94884040	2.45937161	0.11370362
N	-2.07673910	-1.48807085	-0.03783814
H	-1.93501330	-2.47873203	0.07750521
H	-2.98205712	-1.14093829	0.24008660
Si	-2.44569260	1.78780820	-0.40609492
C	-3.88290201	1.57503636	0.92283067
C	-2.09435191	3.71800844	-0.33268690
F	-4.21449219	0.24282812	1.07162622
F	-3.57194380	2.01590701	2.16573059
F	-5.02633687	2.19891253	0.56417851
F	-1.35524644	4.13803929	0.75102548
F	-3.23645228	4.43592573	-0.30472186
F	-1.39492660	4.13219984	-1.42412691

V-SiH_3-T1

E = -1173.5301722 a.u.

C	1.19019788	0.00300870	-0.00326335
C	0.35110838	-1.16010885	0.00228019
C	-0.96254641	0.70031981	0.00228019
C	-0.96254641	-0.73417224	0.00228019
C	0.38378655	1.19095258	-0.00357722
H	0.70200848	-2.18281986	0.00864239
H	-1.84611504	-1.35729519	0.02187342
N	2.55194262	-0.05450488	-0.06004401
H	3.10408927	0.77144319	0.10995876
H	3.00978649	-0.93417295	0.11392176
N	-2.10646311	1.45141123	-0.00238016
H	-2.97809008	0.97858085	0.17773337
H	-2.06889333	2.40492768	0.32444598
Si	1.00650822	2.90625008	-0.21684503
Si	2.77803786	3.51015516	1.20259724
H	3.90976621	2.54464414	1.05311005
H	3.28940491	4.85122789	0.81296128
H	2.44756993	3.54421518	2.65712756
Si	-0.57965946	4.62941689	-0.37157455
H	-1.21084215	4.67298333	-1.71780948
H	-1.70360321	4.53590423	0.61451001
H	0.11111146	5.92440872	-0.13244635

V-H-T1

E = -593.0679898 a.u.

C	-0.96245770	0.69940237	0.00185980
C	-0.96245770	-0.73640440	0.00185980
C	1.18971331	0.00841132	0.00185980
C	0.35389274	-1.15904107	0.00185980
C	0.38130934	1.18763177	-0.00743920
H	-1.84374585	-1.36288345	-0.00688320
H	0.70577707	-2.18145108	-0.00688320
N	-2.09248390	1.46930004	0.03577880
H	-2.01832300	2.44562826	-0.20690420
H	-2.97585393	1.03650217	-0.18177820
N	2.55671347	-0.02340371	0.03577880
H	3.02303743	-0.88954376	-0.18177820
H	3.06475946	0.81361833	-0.20690420
Si	0.93770287	2.92058333	0.16747480
H	2.27644542	3.10019690	-0.47964920
H	-0.04626899	3.84594380	-0.47964920

V-CN-T0

E = -777.1987542 a.u.

C	-0.00001300	1.39121300	1.14212800
C	0.16132500	2.73681000	0.69326900
C	-0.00001300	1.39121300	-1.14212800
C	0.16132500	2.73681000	-0.69326900
C	-0.09472900	0.51635400	0.00000000
H	0.28862400	3.59563400	1.33725900
H	0.28862400	3.59563400	-1.33725900
N	-0.06277700	1.02350900	2.44806300
H	0.05168400	0.05859400	2.72239200
H	0.13658900	1.71031800	3.15730400
N	-0.06277700	1.02350900	-2.44806300
H	0.13658900	1.71031800	-3.15730400
H	0.05168400	0.05859400	-2.72239200
C	0.10200300	-2.08229200	1.49233300
C	0.10200300	-2.08229200	-1.49233300
N	0.40273500	-2.53669900	2.51565600
N	0.40273500	-2.53669900	-2.51565600
Si	-0.59318700	-1.22795100	0.00000000

V-Me-T1

E = -671.5158508 a.u.

C	-0.96013109	0.69656575	0.00173146
C	-0.96013109	-0.74132899	0.00173146
C	1.18613800	0.01147219	0.00173298
C	0.35306366	-1.16050358	0.00173146
C	0.38106052	1.19379463	-0.00692739
H	-1.84301349	-1.36588473	-0.00819912
H	0.71081988	-2.18107340	-0.00819811
N	-2.11133651	1.44068442	0.04759184
H	-2.07202722	2.41289431	-0.21174953
H	-2.97949076	0.97666744	-0.16759149
N	2.55556417	-0.04899392	0.04759790
H	2.99433459	-0.93018003	-0.16757251
H	3.08679408	0.76619627	-0.21174250
Si	0.93787762	2.93810328	0.22518442
C	2.66047010	3.26947718	-0.52892818
H	3.47159374	2.81698849	0.04929028
H	2.73302127	2.92400590	-1.56724568
H	2.84699833	4.34734044	-0.52608614
C	-0.27431968	4.20627268	-0.52855873
H	-0.53378509	3.96686414	-1.56686581
H	-1.19749388	4.30729697	0.04984282
H	0.19810125	5.19288259	-0.52567092

V-NH_2-T1

E = -703.6196077 a.u.

C	1.19338670	0.00335729	-0.00504253
C	0.35388921	-1.15866436	-0.00504031
C	-0.96538504	0.70158106	-0.00504031
C	-0.96538504	-0.73196496	-0.00504031
C	0.38349417	1.18569098	0.02016346
H	0.70221684	-2.18252139	0.00067619
H	-1.84731769	-1.35791254	0.00068092
N	2.55341633	-0.01519565	-0.05013354
H	3.04808922	0.86026832	0.07963366
H	3.05059598	-0.87991022	0.07864401
N	-2.07867471	1.48299135	-0.05011069
H	-2.98807712	1.07321820	0.07863036
H	-1.96696237	2.48232723	0.07961682
Si	0.94042487	2.90759127	-0.17448585
N	-0.32889537	3.93382276	0.51990995
H	-0.46169681	3.90989428	1.52763900
H	-0.37027993	4.89545552	0.20612672
N	2.57018039	2.99613847	0.52015702
H	3.16688343	3.75147542	0.20659723
H	2.66370792	2.89873994	1.52787130

V-Cl-T0

E = -1511.3112280 a.u.

C	-0.98702994	0.67640092	0.00152794
C	0.36130401	1.15325948	0.01334759

C	0.40557978	-1.12558080	-0.01793144
C	1.20717608	0.05873458	0.00152794
C	-0.98702994	-0.76281419	0.00152794
H	0.65087878	2.19431678	0.04930996
H	2.28792922	0.07603846	0.02643492
N	-2.07554061	1.49244669	-0.02250638
H	-2.98891483	1.12097882	0.19370326
H	-1.94371527	2.47808834	0.13618841
N	0.92042135	-2.38420921	-0.06436993
H	1.90905066	-2.50723789	0.08235246
H	0.33288451	-3.17729773	0.14728668
Si	-2.40385506	-1.85405939	-0.34177839
Cl	-2.07416901	-3.76621040	0.53027850
Cl	-4.16182520	-1.06486613	0.55944999

V-OH-T1

E = -743.3514918 a.u.

C	0.39400488	1.12652896	-0.00066595
C	1.20919339	-0.05431400	-0.00028438
C	-0.98516102	-0.67360107	0.00031677
C	0.36712376	-1.15339300	0.00031677
C	-0.98516102	0.75477911	0.00031677
H	2.29025416	-0.06760868	0.02214378
H	0.66131354	-2.19372670	0.02329521
N	0.86849963	2.40702355	-0.00528641
H	0.22419309	3.14083954	0.25973441
H	1.83893915	2.55940482	0.21706026
N	-2.09809377	-1.46503252	-0.00319308
H	-1.99242708	-2.44140416	0.22035617
H	-2.97397894	-1.03370892	0.26259947
Si	-2.41224637	1.84792001	-0.23029882
O	-1.98567960	3.31943799	0.49664827
H	-2.48599320	4.09769987	0.23697802
O	-3.72204364	1.05428579	0.49810269
H	-4.60342855	1.33279504	0.23532133

V-F-T1

E = -791.3677667 a.u.

C	-0.98493400	0.67733571	-0.00975568
C	0.36702075	1.15202670	0.01463352
C	0.39486915	-1.12825396	-0.00975568
C	1.20797809	0.05156258	0.01463352
C	-0.98493400	-0.75267103	-0.00975568
H	0.66342048	2.19091843	0.05716957
H	2.28824486	0.06469768	0.05716957
N	-2.09233148	1.47256036	-0.03265560
H	-2.98854251	1.06956128	0.19923941
H	-1.98853669	2.45758878	0.14886589
N	0.87132418	-2.40563489	-0.03265560
H	1.84903207	-2.56419601	0.14886589
H	0.24708869	-3.16453706	0.19923941
Si	-2.40387275	-1.83700165	-0.33187478
F	-2.10566660	-3.28564348	0.39422916
F	-3.72333466	-1.16878738	0.39422916

VI-CF_3

E = -1266.0338704a.u.

C	0.22802740	-1.39295180	0.01390160
C	-0.95921660	-0.73919180	0.08446860
C	0.22659240	1.39099520	-0.05126740
C	-0.96155860	0.74060420	0.01133260
H	-1.90410160	-1.26228180	0.19981460
H	-1.91324760	1.26364420	-0.02231640
N	0.43461640	-2.75907680	0.05424660
H	1.37571540	-3.09366980	0.17537960
H	-0.27228260	-3.32223880	0.50374860
N	0.44114940	2.74103720	-0.28656640
H	-0.36531960	3.34045220	-0.17512940
H	1.28616940	3.13793220	0.09453860
C	3.20358740	0.00504420	-0.01917740
Si	1.46615540	0.00054420	-0.05843540
C	4.00756640	-1.24683680	-0.09531540
C	3.99359140	1.26563720	0.08103960
F	5.03290840	-1.17355180	-0.97141340
F	4.55055040	-1.62149780	1.09104060
F	3.23537640	-2.30626280	-0.49499140
F	5.02546840	1.17782620	0.94874260
F	4.52399140	1.67673120	-1.09683940
F	3.21504840	2.30643120	0.51773660

VI-SiH_3

E = -1173.5538228 a.u.

C	0.22407700	-1.38101680	-0.01026800
C	-0.96898000	-0.74065080	0.03202500
C	0.22427500	1.38097320	-0.01027500
C	-0.96888000	0.74081620	0.03153700
H	-1.91813000	-1.26981980	0.05424300
H	-1.91799900	1.27012520	0.05203800
N	0.43232300	-2.75413680	-0.11038300
H	1.31569100	-3.10236280	0.22985000
H	-0.34701800	-3.33773980	0.16375500
N	0.43299800	2.75386620	-0.11349100

H	-0.34772800	3.33794820	0.15574100
H	1.31451800	3.10293720	0.23077900
C	3.20773400	-0.00008380	-0.01789700
Si	1.48950800	-0.00012180	-0.04301900
Si	4.18962300	1.57666220	-0.00055100
H	3.31903500	2.77132620	0.18315100
H	5.17504500	1.57449120	1.11539800
H	4.95347900	1.77597220	-1.26283000
Si	4.19024100	-1.57641580	-0.00360200
H	3.31944000	-2.77226280	0.17108300
H	4.95895700	-1.76960180	-1.26389200
H	5.17142700	-1.57910780	1.11606500

VI-H

E = -593.0769272 a.u.

C	1.37727200	0.22679360	0.01942080
C	0.74095400	-0.96861940	-0.04467420
C	-1.37727200	0.22679360	0.01942080
C	-0.74095400	-0.96861940	-0.04467420
H	1.27123000	-1.91633740	-0.09495620
H	-1.27123000	-1.91633740	-0.09495620
N	2.75301400	0.45743260	-0.04467420
H	3.08292600	1.27760460	0.44283080
H	3.33489300	-0.34765240	0.14969980
N	-2.75301400	0.45743260	-0.04467420
H	-3.33489300	-0.34765240	0.14969980
H	-3.08292600	1.27760460	0.44283080
C	0.00000000	3.19019060	0.14373280
Si	0.00000000	1.48365160	0.05050680
H	-0.91441900	3.77289360	0.15697080
H	0.91441900	3.77289360	0.15697080

VI-CN

E = -777.1764486 a.u.

C	0.01014400	-1.36174600	1.39673700
C	-0.08064500	-2.54975900	0.74496100
C	0.01014400	-1.36174600	-1.39673700
C	-0.08064500	-2.54975900	-0.74496100
C	0.01763100	1.59152900	0.00000000
H	-0.14740500	-3.50015800	1.26621300
H	-0.14740500	-3.50015800	-1.26621300
N	0.10944100	-1.11382400	2.75497800
H	-0.12749000	-0.18909700	3.08238200
H	-0.18863300	-1.85032900	3.37913100
N	0.10944100	-1.11382400	-2.75497800
H	-0.18863300	-1.85032900	-3.37913100
H	-0.12749000	-0.18909700	-3.08238200
C	-0.01614900	2.28478900	1.23533800
C	-0.01614900	2.28478900	-1.23533800
N	-0.04994400	2.77304300	2.28621100
N	-0.04994400	2.77304300	-2.28621100
Si	0.07343700	-0.15560600	0.00000000

VI-Me

E = -671.5050292 a.u.

C	0.22734820	-1.37732940	0.02384960
C	-0.96895780	-0.73831940	-0.03626040
C	0.22731920	1.37733560	0.02384360
C	-0.96897180	0.73829960	-0.03625940
H	-1.91616780	-1.27082940	-0.07766140
H	-1.91619280	1.27079160	-0.07764540
N	0.43904220	-2.76099240	-0.03643440
H	1.21252520	-3.10211640	0.51647560
H	-0.39109480	-3.31842640	0.12561560
N	0.43898720	2.76100560	-0.03642440
H	-0.39116480	3.31841560	0.12563660
H	1.21245520	3.10213460	0.51650560
C	3.21056420	0.00002360	0.00229660
Si	1.48326220	0.00001360	0.02482660
C	4.02616120	-1.27020040	-0.02088740
H	4.67408920	-1.33832240	0.86376960
H	3.41704220	-2.17633240	-0.05913140
H	4.68899320	-1.28787040	-0.89654040
C	4.02614220	1.27025960	-0.02091340
H	3.41700820	2.17638060	-0.05918440
H	4.67406220	1.33841460	0.86374660
H	4.68898120	1.28791860	-0.89656140

VI-NH_2

E = -703.5838033 a.u.

C	-1.10119365	0.77116347	0.02953896
C	-1.10119365	-0.58380308	0.02953896
C	1.28647855	-0.38997705	0.02932693
C	0.22076758	-1.22672918	0.02953896
H	-2.00882184	-1.18764325	0.04679770
H	0.30613682	-2.31351267	0.04754233
N	-2.22764513	1.61524733	0.21385116
H	-2.25662410	2.38424355	-0.44711219
H	-3.11659903	1.12276381	0.19413185
N	2.64592069	-0.75454205	0.21488385
H	2.80816753	-1.75771779	0.19369727
H	3.26945097	-0.30070155	-0.44412801

C	0.85125892	1.75015067	1.78356354
Si	0.69514117	1.42934585	-0.11794381
N	1.96266498	1.40060901	2.44226407
H	2.07195500	1.54054271	3.43769867
H	2.58434007	0.73400468	1.99022290
N	-0.10806292	2.41280050	2.44095825
H	-0.06645037	2.58420573	3.43660001
H	-1.01546942	2.49293347	1.98790928

VI-Cl

E = -1511.2040500 a.u.

C	-1.10943716	0.86760320	-0.00221023
C	-1.10943716	-0.49109425	-0.00221023
C	1.33185180	-0.45799223	-0.00221023
C	0.19231306	-1.19793157	-0.00221023
H	-2.02600365	-1.07463623	0.00086682
H	0.20205395	-2.28444918	0.00086682
N	-2.20253366	1.72560051	0.07684874
H	-2.06980916	2.65162426	-0.30188119
H	-3.09319517	1.32674993	-0.18900996
N	2.64674813	-0.90751088	0.07684874
H	2.79728186	-1.87172004	-0.18900996
H	3.35112264	-0.29188736	-0.30188119
C	1.51595045	2.79185716	-0.15608332
Si	0.69470944	1.27941486	0.00884091
Cl	3.26436489	2.91816001	-0.22235424
Cl	0.66970345	4.32703516	-0.22235424

VI-OH

E = -743.2398200 a.u.

C	-1.10725781	0.85892966	-0.01129784
C	-1.10725781	-0.50074074	-0.01129784
C	1.32755947	-0.44951560	-0.01767957
C	0.19350470	-1.20005572	-0.01129784
H	-2.02403318	-1.08514463	-0.01585270
H	0.21220946	-2.28702934	-0.00649813
N	-2.21348593	1.71142461	0.05786976
H	-2.08799844	2.60683675	-0.39298779
H	-3.09260610	1.28567969	-0.20820951
N	2.64626924	-0.90456211	0.05431531
H	2.79085248	-1.85686180	-0.25551552
H	3.34286966	-0.27793804	-0.32129772
C	1.45786068	2.75244921	-0.53115196
Si	0.69345145	1.29138240	0.05157311
O	2.82828517	2.90326428	-0.55559144
H	3.08376821	3.26349190	-1.41772590
O	0.75590432	3.89556209	-0.82181013
H	1.13006102	4.63699216	-0.32089568

VI-F

E = -791.2201981 a.u.

C	-1.10803587	0.86601800	-0.02153256
C	-1.10803587	-0.49302038	-0.02153256
C	1.32957027	-0.45822872	-0.02153256
C	0.18944039	-1.19788352	-0.02153256
H	-2.02639021	-1.07447802	-0.02781066
H	0.20145473	-2.28477051	-0.02781066
N	-2.21115539	1.71730513	0.05357488
H	-2.09758542	2.61976801	-0.38529849
H	-3.09463660	1.29264052	-0.19865012
N	2.64410674	-0.92035028	0.05357488
H	2.76867887	-1.89264697	-0.19865012
H	3.33939418	-0.33390952	-0.38529849
F	2.77202629	2.81887480	-0.85739001
F	0.85615010	3.85968806	-0.85739001
C	1.45432018	2.67703874	-0.66628817
Si	0.69706107	1.28311463	0.08613027

VI-CF_3-T1

E = -1266.005344 a.u.

C	0.26042520	-1.33109140	0.01451440
C	-1.02270480	-0.69194140	0.00067340
C	0.26216820	1.33068960	-0.01761560
C	-1.02181180	0.69307860	-0.01952060
H	-1.94242380	-1.26737240	0.00859040
H	-1.94076080	1.26960360	-0.03447560
N	0.39468820	-2.67894840	0.04871540
H	1.30471620	-3.10660340	-0.00998160
H	-0.41240680	-3.28124040	0.00157740
N	0.39873620	2.67811160	-0.05400260
H	-0.40789480	3.28222860	-0.02745060
H	1.30910920	3.10493460	0.00475840
C	3.28604620	-0.00091540	-0.00060060
Si	1.52192320	-0.00073540	0.02194840
C	4.05515720	-1.25637340	-0.02599260
C	4.05435120	1.25519660	0.02009640
F	5.06380520	-1.27674040	-0.93084060
F	4.63234120	-1.60623140	1.16019840
F	3.23807820	-2.32718340	-0.34505260
F	5.07362420	1.27530360	0.91300040
F	4.61685120	1.60848660	-1.17195260
F	3.23946620	2.32409060	0.35182140

VI-SiH_3-T1

E = -1173.5180483 a.u.

C	0.26005340	-1.32265100	0.00841300
C	-1.02954860	-0.69158700	0.00465200
C	0.26008240	1.32264700	-0.00839300
C	-1.02953360	0.69160100	-0.00500600
H	-1.94770060	-1.27039300	0.01152900
H	-1.94767460	1.27042500	-0.01203500
N	0.39025740	-2.67724000	0.03572600
H	1.29816740	-3.11028200	-0.01683600
H	-0.41669160	-3.27839600	-0.02627100
N	0.39031040	2.67722200	-0.03536200
H	-0.41669460	3.27846800	0.02490800
H	1.29823440	3.11033100	0.01629000
C	3.28088240	-0.00001500	0.00002400
Si	1.53894640	-0.00001000	0.00033400
Si	4.21791140	1.58203300	0.02161900
H	3.29382240	2.75962100	0.06766300
H	5.11838240	1.71707100	1.20376100
H	5.07824740	1.77910400	-1.18155900
Si	4.21789340	-1.58207300	-0.02175700
H	3.29379640	-2.75963000	-0.06838200
H	5.11862140	-1.71668800	-1.20374900
H	5.07797040	-1.77958700	1.18153600

VI-H-T1

E = -593.0320172 a.u.

C	1.31930200	0.26465560	0.01187700
C	0.68937200	-1.03263740	-0.01283900
C	-1.31930200	0.26465560	0.01187700
C	-0.68937200	-1.03263740	-0.01283900
H	1.27107400	-1.94880340	-0.03813800
H	-1.27107400	-1.94880340	-0.03813800
N	2.68430300	0.38928360	-0.01283900
H	3.10822800	1.28111760	0.18411200
H	3.25974500	-0.41500940	0.18937100
N	-2.68430300	0.38928360	-0.01283900
H	-3.25974500	-0.41500940	0.18937100
H	-3.10822800	1.28111760	0.18411200
C	0.00000000	3.26835560	0.08242800
Si	0.00000000	1.53596360	0.00192400
H	-0.91582700	3.84755560	0.08503400
H	0.91582700	3.84755560	0.08503400

VI-CN-T1

E = -777.1539777 a.u.

C	0.04876200	-1.25983800	1.32703100
C	-0.32632300	-2.46910600	0.70189900
C	0.04876200	-1.25983800	-1.32703100
C	-0.32632300	-2.46910600	-0.70189900
C	0.04685400	1.56099500	0.00000000
H	-0.61315800	-3.35193800	1.26664900
H	-0.61315800	-3.35193800	-1.26664900
N	-0.01360600	-1.04806300	2.65207400
H	0.13745300	-0.12260500	3.03058100
H	-0.42782000	-1.72936300	3.27282500
N	-0.01360600	-1.04806300	-2.65207400
H	-0.42782000	-1.72936300	-3.27282500
H	0.13745300	-0.12260500	-3.03058100
C	-0.14632200	2.18598700	1.23936800
C	-0.14632200	2.18598700	-1.23936800
N	-0.27854300	2.56510900	2.33265100
N	-0.27854300	2.56510900	-2.33265100
Si	0.76447300	-0.12009500	0.00000000

VI-Me-T1

E = -671.4560643 a.u.

C	-1.07310676	0.80080174	0.05675232
C	-1.07310676	-0.62753520	0.05675232
C	1.29421674	-0.34322318	0.05674640
C	0.17503739	-1.23071451	0.05675232
H	-1.99251815	-1.20508318	0.00129806
H	0.29378731	-2.30996585	0.00136240
N	-2.24336749	1.49285399	0.13108988
H	-2.26153712	2.49068230	0.00799386
H	-3.13133135	1.01776923	0.06236018
N	2.56357927	-0.83022599	0.13155374
H	2.74297434	-1.82115323	0.06220661
H	3.35668969	-0.22454868	0.00790976
C	1.34841377	2.78985263	0.72409916
Si	0.67695938	1.40067116	-0.22700338
C	0.54715263	4.04081472	0.97171697
H	0.86871846	4.88075766	0.33470143
H	-0.52728468	3.90822570	0.81163770
H	0.67324366	4.37830535	2.01101820
C	2.82659094	2.93967130	0.97066250
H	3.39047023	2.01567103	0.80977570
H	3.28417885	3.71390026	0.33357952
H	3.01338377	3.24782800	2.00993832

VI-NH_2-T1

E = -703.5060997 a.u.

C	0.49434794	1.22989278	0.09089943
C	1.24795449	0.02926029	0.09089943
C	-0.91129062	-0.95911207	0.07110971
C	0.49434794	-1.14697309	0.09089943
H	2.33594878	0.01541438	0.06616009
H	0.95951269	-2.13015037	0.07554365
N	1.08357725	2.44172818	0.20567272
H	0.52743806	3.28071458	0.23369560
H	2.07921938	2.54386789	0.33531894
N	-1.77687186	-1.99473478	0.18360034
H	-1.45624398	-2.93007751	0.38799492
H	-2.75809450	-1.80484969	0.32212008
C	-2.50915186	1.47125659	0.97402082
Si	-1.32535975	0.84693208	-0.34380801
N	-3.21107168	0.54229565	1.80254398
H	-2.62644737	0.09220468	2.49733622
H	-4.05107609	0.91563338	2.23251611
N	-3.15086829	2.71483413	0.74100327
H	-3.59267227	2.83146425	-0.16679471
H	-3.76335277	3.03066306	1.48448432

VI-Cl-T1

E = -1511.1644056 a.u.

C	0.87169170	-1.08609517	-0.01724588
C	-0.48368329	-1.12374463	-0.01724588
C	-0.48368329	1.30601211	-0.01724588
C	-1.21181342	0.16175839	-0.01721064
H	-1.04572861	-2.05505294	-0.01976264
H	-2.29958632	0.15825147	-0.02059863
N	1.74933962	-2.16574188	-0.10758435
H	2.64802757	-2.04734451	0.33633892
H	1.34821183	-3.07314349	0.09285994
N	-0.96233312	2.61312051	-0.10508422
H	-1.94465825	2.73346914	0.10713577
H	-0.39572558	3.32469814	0.33225491
C	2.49165668	1.41393203	-1.20138254
Si	1.30748830	0.74206930	0.06894828
Cl	3.95608288	2.23885403	-0.75911309
Cl	2.21261876	1.25563299	-2.90770652

VI-OH-T1

E = -743.2061601 a.u.

C	-1.09680108	0.81806291	-0.04989888
C	-1.09680108	-0.53763728	-0.04989888
C	1.30652574	-0.44080892	0.10469478
C	0.20497658	-1.22093841	-0.04989888
H	-2.01100442	-1.12589947	0.02424665
H	0.25293332	-2.29900974	-0.18674440
N	-2.20772674	1.65503539	0.26884195
H	-2.32240509	2.42858597	-0.37775544
H	-3.08503925	1.14552044	0.32674436
N	2.62274205	-0.85637316	0.13811913
H	2.84825289	-1.76367534	-0.24598792
H	3.33868147	-0.16262030	-0.00620712
C	0.60619114	2.71083185	1.36501864
Si	0.68209983	1.38132171	0.04500188
O	1.71211334	3.39207829	1.76996974
H	1.46816982	3.92805038	2.53793846
O	-0.36493181	2.69044290	2.32787341
H	-1.20085169	2.40391520	1.90056219

VI-F-T1

E = -791.1909548 a.u.

C	-1.07794959	0.77715216	0.07351400
C	-1.07794959	-0.63297391	0.07351400
C	1.28232478	-0.34868892	0.07351400
C	0.18642160	-1.23607373	0.07351400
H	-1.99219503	-1.22228081	0.06189600
H	0.30376162	-2.31744262	0.06189600
N	-2.21290747	1.49653909	0.16732300
H	-2.18316741	2.50307921	0.20165300
H	-3.11162126	1.06039258	0.31576200
N	2.55563134	-0.77803417	0.16732300
H	2.78222854	-1.75094935	0.31576200
H	3.31916564	-0.12151085	0.20165300
F	2.43979436	2.56222153	1.59649100
F	0.45592396	3.50851950	1.59649100
C	1.11426864	2.33601325	1.35475500
Si	0.68715279	1.44058441	-0.29405600

15

E = -2251.9506203 a.u.

C	0.000074000	1.179355000	-0.141681000
C	0.000048000	0.740295000	-1.420188000
C	-0.000074000	-1.179355000	-0.141681000
C	-0.000048000	-0.740295000	-1.420188000
C	0.000000000	0.000000000	0.752085000
C	0.000000000	0.000000000	2.116556000
C	-0.000012000	-1.183875000	2.922547000

C	0.000012000	1.183875000	2.922547000
N	0.000000000	-2.065201000	3.669117000
N	0.000000000	2.065201000	3.669117000
Cl	-0.000143000	-1.686655000	-2.839798000
Cl	-0.000232000	-2.826752000	0.342515000
Cl	0.000143000	1.686655000	-2.839798000
Cl	0.000232000	2.826752000	0.342515000

15h

E = -2252.248896 a.u.

C	0.270178000	1.195707000	-0.000017000
C	1.521878000	0.678664000	-0.000013000
C	0.115541000	-1.167251000	0.000013000
C	1.423698000	-0.827267000	-0.000001000
C	-0.676593000	0.068124000	0.000001000
C	-2.053872000	0.160337000	0.000008000
C	-2.908162000	-0.962601000	0.000072000
C	-2.827405000	1.363473000	-0.000042000
N	-3.751604000	-1.742291000	0.000128000
N	-3.563509000	2.253540000	-0.000083000
Cl	2.761535000	-1.849432000	-0.000017000
Cl	-0.523693000	-2.762583000	0.000000000
Cl	2.986076000	1.511016000	-0.000008000
Cl	-0.137263000	2.855545000	-0.000010000
H	-4.458927000	-2.461151000	0.000166000

15h2

E = -2252.4331763 a.u.

C	0.103270000	1.142260000	-0.000249000
C	1.577048000	0.675800000	-0.000168000
C	0.205185000	-1.099842000	0.000152000
C	1.586930000	-0.690906000	0.000125000
C	-0.710331000	0.046530000	-0.000050000
C	-2.192553000	-0.006273000	-0.000013000
C	-2.907200000	-0.025477000	1.181504000
C	-2.907240000	-0.026432000	-1.181481000
N	-3.479015000	-0.094204000	2.182547000
N	-3.479040000	-0.095726000	-2.182501000
Cl	2.925112000	-1.733014000	0.000377000
Cl	-0.290023000	-2.678367000	0.000540000
Cl	2.868548000	1.720329000	-0.000336000
Cl	-0.317932000	2.754637000	-0.000544000
H	-3.990565000	0.078010000	3.037844000
H	-3.990702000	0.076593000	-3.037711000

15-T1

E = -2251.9124602 a.u.

C	0.000006000	1.130228000	-0.105236000
C	0.000000000	0.685519000	-1.482270000
C	-0.000006000	-1.130228000	-0.105236000
C	0.000000000	-0.685519000	-1.482270000
C	0.000000000	0.000000000	0.775611000
C	0.000000000	0.000000000	2.194629000
C	0.000922000	-1.183888000	2.972846000
C	-0.000922000	1.183888000	2.972846000
N	0.001731000	-2.108321000	3.672345000
N	-0.001731000	2.108321000	3.672345000
Cl	-0.000031000	-1.714243000	-2.845157000
Cl	-0.000252000	-2.772833000	0.319911000
Cl	0.000031000	1.714243000	-2.845157000
Cl	0.000252000	2.772833000	0.319911000

15h-T1

E = -2252.2281212 a.u.

C	-0.208100000	1.150200000	-0.002849000
C	-1.548844000	0.641239000	-0.003864000
C	-0.106380000	-1.129069000	0.008664000
C	-1.482848000	-0.758804000	0.003388000
C	0.717294000	0.047376000	0.004588000
C	2.137663000	0.116161000	0.006116000
C	2.969062000	-0.979759000	-0.015125000
C	2.879360000	1.335515000	0.040598000
N	3.770809000	-1.820539000	-0.160657000
N	3.549448000	2.276614000	0.071507000
Cl	-2.791743000	-1.825629000	0.007476000
Cl	0.428759000	-2.735542000	0.026610000
Cl	-2.952173000	1.575530000	-0.013758000
Cl	0.153005000	2.793937000	-0.017738000
H	4.371534000	-2.470697000	0.330913000

15h2-T0

E = -2252.434136 a.u.

C	0.000000000	1.145721000	-0.187015000
C	-0.000817000	0.714246000	-1.549661000
C	0.000000000	-1.145721000	-0.187015000
C	0.000817000	-0.714246000	-1.549661000
C	0.000000000	0.000000000	0.668613000
C	0.000000000	0.000000000	2.123119000
C	0.567680000	-1.018775000	2.882590000
C	-0.567680000	1.018775000	2.882590000
N	1.050315000	-1.821047000	3.551130000
N	-1.050315000	1.821047000	3.551130000
Cl	-0.013772000	-1.699734000	-2.896680000

Cl	-0.055940000	-2.760769000	0.294249000
Cl	0.013772000	1.699734000	-2.896680000
Cl	0.055940000	2.760769000	0.294249000
H	1.468567000	-2.536439000	4.132732000
H	-1.468567000	2.536439000	4.132732000

15'

E = -2502.9784258 a.u.

C	0.416187000	1.165792000	0.000068000
C	1.704921000	0.734030000	0.000438000
C	0.415867000	-1.165556000	-0.001353000
C	1.704716000	-0.734144000	-0.000713000
C	-0.466250000	0.000268000	-0.000982000
C	-3.235619000	-1.484571000	0.004504000
C	-3.236575000	1.484352000	-0.005242000
N	-3.958561000	-2.387751000	0.013232000
N	-3.959560000	2.387536000	-0.007829000
Cl	3.120615000	-1.697283000	-0.001340000
Cl	-0.109230000	-2.810932000	-0.003538000
Cl	3.121080000	1.696779000	0.002681000
Cl	-0.108513000	2.811271000	0.002903000
Si	-2.199988000	0.000234000	-0.002151000

15h'

E = -2503.2725064 a.u.

C	-0.396550000	-1.149467000	0.067574000
C	-1.704191000	-0.792895000	-0.003752000
C	-0.513032000	1.195399000	0.052203000
C	-1.778704000	0.708363000	-0.014570000
C	0.409064000	0.063820000	0.066879000
C	3.106921000	-1.339361000	-0.110992000
C	3.233322000	1.555270000	-0.079303000
N	3.823817000	-2.217172000	-0.306823000
N	3.998535000	2.396908000	-0.294542000
Cl	-3.223979000	1.575083000	-0.117394000
Cl	-0.031219000	2.844557000	0.076782000
Cl	-3.055131000	-1.801788000	-0.089167000
Cl	0.230905000	-2.755812000	0.119716000
Si	2.144425000	0.188660000	0.358023000
H	4.430816000	-3.000853000	-0.499932000

15h2'

E = -2503.4859947 a.u.

C	-0.009508000	0.910896000	-0.000090000
C	-1.551081000	0.955252000	-0.000006000
C	-0.804401000	-1.158451000	-0.000146000
C	-1.994043000	-0.332742000	-0.000043000
C	0.440835000	-0.381516000	-0.000094000
C	3.039954000	-0.179268000	-1.389770000
C	3.039808000	-0.179642000	1.389889000
N	3.626191000	0.146270000	-2.325754000
N	3.625942000	0.145558000	2.326054000
Cl	-3.591792000	-0.899657000	0.000022000
Cl	-0.869851000	-2.814900000	-0.000185000
Cl	-2.444576000	2.360852000	0.000134000
Cl	0.884033000	2.328661000	0.000067000
H	4.150883000	0.421849000	-3.146497000
H	4.150460000	0.420087000	3.147259000
Si	2.167251000	-1.233296000	-0.000139000

15'-T1

E = -2502.958101 a.u.

C	-0.359182000	-1.118637000	-0.109055000
C	-1.734774000	-0.683908000	0.027352000
C	-0.356458000	1.118630000	-0.105745000
C	-1.733158000	0.686729000	0.029412000
C	0.513513000	-0.000954000	-0.163659000
C	3.188126000	1.469798000	0.187475000
C	3.184518000	-1.473290000	0.204103000
N	3.797438000	2.403391000	0.500598000
N	3.790633000	-2.405112000	0.528496000
Cl	-3.085214000	1.723836000	0.173201000
Cl	0.095374000	2.759111000	-0.192295000
Cl	-3.089451000	-1.718107000	0.168075000
Cl	0.089043000	-2.759867000	-0.200719000
Si	2.321587000	-0.004480000	-0.481673000

15h'-T1

E = -2503.2673946 a.u.

C	0.377245000	-1.111774000	-0.165483000
C	1.743940000	-0.724314000	0.010152000
C	0.429880000	1.143783000	-0.095912000
C	1.779028000	0.667687000	0.053492000
C	-0.469061000	0.035899000	-0.189348000
C	-3.114683000	-1.303299000	0.350577000
C	-3.159610000	1.515977000	0.057038000
N	-3.780324000	-2.150600000	0.758066000
N	-3.819352000	2.411025000	0.379446000
Cl	3.148861000	1.639652000	0.263927000
Cl	0.011325000	2.782422000	-0.141724000
Cl	3.062937000	-1.779158000	0.156717000
Cl	-0.138315000	-2.727687000	-0.317778000
Si	-2.243136000	0.082570000	-0.611811000

H	-4.360513000	-2.881597000	1.140236000

15h2'-T1

E = -2503.4823175 a.u.

C	0.421467000	1.135492000	0.147153000
C	1.772313000	0.715233000	-0.053738000
C	0.422371000	-1.135462000	0.147513000
C	1.772856000	-0.714316000	-0.053566000
C	-0.442168000	-0.000350000	0.227286000
C	-3.042920000	1.373142000	-0.271034000
C	-3.041789000	-1.373943000	-0.272730000
N	-3.671374000	2.238983000	-0.691996000
N	-3.669048000	-2.240031000	-0.694987000
Cl	3.105832000	-1.700777000	-0.256076000
Cl	-0.047167000	-2.755632000	0.285028000
Cl	3.104533000	1.702660000	-0.256397000
Cl	-0.049172000	2.755333000	0.284101000
H	-4.217256000	3.005302000	-1.068496000
H	-4.214252000	-3.006271000	-1.072637000
Si	-2.235483000	-0.001241000	0.832970000

V-CN'

E = -777.5684008 a.u.

C	-1.768795000	-0.811953000	-0.276530000
C	-2.923222000	-0.027466000	0.275086000
C	-0.962489000	1.136419000	0.424735000
C	-2.440412000	1.139382000	0.697166000
C	-0.561313000	-0.097285000	-0.145931000
H	-3.947477000	-0.372738000	0.299058000
H	-2.982141000	1.963072000	1.141323000
N	-1.951815000	-2.005020000	-0.815495000
H	-1.177090000	-2.510247000	-1.231323000
H	-2.870857000	-2.417510000	-0.890304000
N	-0.226664000	2.195539000	0.682896000
H	-0.641376000	3.038853000	1.055765000
H	0.748260000	2.243099000	0.391825000
C	1.992464000	-1.121254000	0.861901000
C	2.005681000	0.904272000	-0.989420000
N	2.587191000	-1.604026000	1.730528000
N	2.493869000	1.945599000	-1.133469000
Si	1.098079000	-0.741332000	-0.826109000
H	3.128029000	-2.023212000	2.465910000

V-CN''

E = -777.5227055 a.u.

C	-0.603758051	1.611938709	1.083407421
C	-0.069088103	2.904418457	0.558796025
C	0.667908574	1.145645645	-0.700495023
C	0.687622125	2.627058219	-0.502687029
C	-0.136132683	0.518366714	0.287854285
H	-0.280077996	3.873887375	0.989857356
H	1.230960946	3.321483172	-1.129544480
N	-1.387418920	1.591132528	2.135941282
H	-1.646449347	2.446692784	2.614411052
H	-1.767442095	0.731216657	2.517625131
N	1.339517166	0.595529509	-1.688790322
H	1.346108767	-0.403169143	-1.849022563
H	1.881367490	1.159176321	-2.333499775
C	1.035733711	-2.225553718	0.647850121
C	-1.199717442	-1.974350256	-1.010987551
N	1.942940782	-2.879587725	0.929298920
N	-1.814378408	-2.457343132	-1.858871948
Si	-0.630745096	-1.238449539	0.688419717
H	2.721021858	-3.466376337	1.200467133
H	-2.373537707	-2.893846633	-2.580029755

V-CN'-T1

E = -777.52270558 a.u.

C	-1.610543914	-0.987304414	-0.228358348
C	-2.810453337	-0.425559475	0.255031297
C	-1.244138481	1.250681620	0.214894700
C	-2.593878065	0.932419610	0.516674554
C	-0.566546741	0.028087064	-0.201099027
H	-3.744429802	-0.954246410	0.381967402
H	-3.327215738	1.630990788	0.894266052
N	-1.434481558	-2.272914193	-0.622232608
H	-0.686210111	-2.513035048	-1.256432221
H	-2.238344541	-2.882816405	-0.665657898
N	-0.695593683	2.468770704	0.336052706
H	-1.253231587	3.246001313	0.657405120
H	0.285338788	2.645945693	0.170610436
C	1.877934966	-1.422127158	0.509779987
C	2.147755476	1.257356360	-0.328566320
N	2.371685248	-2.259048410	1.133965211
N	2.725831412	2.245752885	-0.155056006
Si	1.155922453	-0.235403571	-0.798232653
H	2.808309269	-2.956438496	1.713852034

V-CN''-T1

E = -777.7383992 a.u.

C	0.045071162	-1.469604793	1.161385382
C	-0.596107561	-2.640032656	0.704610244
C	0.045071162	-1.469604793	-1.161385382

C	-0.596107561	-2.640032656	-0.704610244
C	0.333806841	-0.630331412	0.000000000
H	-0.982995430	-3.430140660	1.333823144
H	-0.982995430	-3.430140660	-1.333823144
N	0.294886782	-1.153439469	2.449208678
H	1.050096634	-0.531433925	2.701644472
H	0.056899683	-1.825488833	3.168812334
N	0.294886782	-1.153439469	-2.449208678
H	0.056899683	-1.825488833	-3.168812334
H	1.050096634	-0.531433925	-2.701644472
C	-0.179385342	1.937342986	1.365822482
C	-0.179385342	1.937342986	-1.365822482
N	-0.628565732	2.526988949	2.245496943
N	-0.628565732	2.526988949	-2.245496943
Si	0.947472793	1.150078701	0.000000000
H	-1.039447879	3.046427130	3.012306358
H	-1.039447879	3.046427130	-3.012306358

P-CN

E = -526.1686633 a.u.

C	-0.017837000	-1.173367000	1.199670000
C	-0.040499000	-2.443809000	0.739086000
C	-0.017837000	-1.173367000	-1.199670000
C	-0.040499000	-2.443809000	-0.739086000
C	0.006172000	-0.277983000	0.000000000
H	-0.055072000	-3.336433000	1.348908000
H	-0.055072000	-3.336433000	-1.348908000
N	0.112585000	-0.723172000	2.510916000
H	-0.411361000	0.098991000	2.777096000
H	0.029460000	-1.455345000	3.202252000
N	0.112585000	-0.723172000	-2.510916000
H	0.029460000	-1.455345000	-3.202252000
H	-0.411361000	0.098991000	-2.777096000
C	0.015396000	1.873057000	1.194852000
C	0.015396000	1.873057000	-1.194852000
N	-0.028986000	2.543204000	2.134821000
N	-0.028986000	2.543204000	-2.134821000
C	0.030299000	1.083742000	0.000000000

P-CN'

E = -526.5311432 a.u.

C	-1.039687000	-1.170891000	0.275693000
C	-2.499725000	-0.859064000	0.106014000
C	-1.206977000	0.979687000	-0.319495000
C	-2.599564000	0.422639000	-0.239906000
C	-0.273392000	-0.035684000	-0.026604000
H	-3.297694000	-1.571889000	0.258950000
H	-3.496787000	0.994097000	-0.431028000
N	-0.620738000	-2.357698000	0.673738000
H	0.361355000	-2.553297000	0.825267000
H	-1.272870000	-3.099796000	0.887606000
N	-0.973986000	2.244637000	-0.596148000
H	-1.732917000	2.892861000	-0.759840000
H	-0.035726000	2.632308000	-0.567486000
C	2.012152000	-0.829387000	-0.472856000
C	1.745942000	1.302418000	0.561704000
N	2.703378000	-1.776424000	-0.747561000
N	2.083218000	2.337644000	0.953863000
C	1.194907000	0.102622000	0.026211000
H	3.129597000	-1.905441000	-1.665281000

P-CN''

E = -526.7537911 a.u.

C	-1.181458000	-1.113884000	-0.172807000
C	-2.604447000	-0.658627000	-0.101803000
C	-1.181035000	1.114101000	0.172759000
C	-2.604284000	0.659246000	0.101960000
C	-0.322889000	-0.000083000	0.000016000
H	-3.458957000	-1.314085000	-0.202824000
H	-3.458582000	1.314954000	0.203153000
N	-0.866482000	-2.372861000	-0.367950000
H	0.094122000	-2.691256000	-0.416555000
H	-1.581682000	-3.083352000	-0.477145000
N	-0.865574000	2.372955000	0.367790000
H	-1.580488000	3.083724000	0.477064000
H	0.095157000	2.691044000	0.415839000
C	1.877248000	-0.234174000	1.159767000
C	1.877274000	0.233554000	-1.159836000
N	2.432003000	-0.505573000	2.138961000
N	2.432232000	0.505845000	-2.138760000
C	1.161940000	-0.000360000	-0.000110000
H	2.915298000	-0.439976000	3.024577000
H	2.915780000	0.437753000	-3.024069000

P-CN-T1

E = -526.1602902 a.u.

C	-0.000039000	-1.128940000	1.149670000
C	0.000019000	-2.480180000	0.693037000
C	-0.000039000	-1.128940000	-1.149670000
C	0.000019000	-2.480180000	-0.693037000
C	-0.000036000	-0.250782000	0.000000000
H	0.000095000	-3.348805000	1.335721000

H	0.000095000	-3.348805000	-1.335721000
N	-0.000058000	-0.764571000	2.452261000
H	0.000032000	0.201814000	2.743362000
H	0.000219000	-1.470713000	3.169094000
N	-0.000058000	-0.764571000	-2.452261000
H	0.000219000	-1.470713000	-3.169094000
H	0.000032000	0.201814000	-2.743362000
C	0.000019000	1.914010000	1.199829000
C	0.000019000	1.914010000	-1.199829000
N	0.000016000	2.483399000	2.212647000
N	0.000016000	2.483399000	-2.212647000
C	0.000019000	1.169639000	0.000000000

P-CN'-T1

E = -526.4957404 a.u.

C	1.032932000	-1.293285000	-0.101307000
C	2.407587000	-1.012800000	0.022620000
C	1.323940000	1.011572000	0.080507000
C	2.585563000	0.371964000	0.128430000
C	0.304792000	-0.029444000	-0.031942000
H	3.196500000	-1.750799000	0.005252000
H	3.533545000	0.882035000	0.221685000
N	0.490232000	-2.517592000	-0.260342000
H	-0.455173000	-2.652704000	-0.582051000
H	1.100036000	-3.317177000	-0.354294000
N	1.123952000	2.334067000	0.158703000
H	1.913727000	2.956832000	0.248149000
H	0.210974000	2.760411000	0.081543000
C	-2.010585000	-0.841108000	0.193770000
C	-1.691750000	1.453739000	-0.173108000
N	-2.814253000	-1.717021000	0.221170000
N	-2.117722000	2.521126000	-0.293083000
C	-1.111627000	0.156071000	-0.020979000
H	-3.320183000	-2.122905000	1.006635000

P-CN''-T1

E = -526.6954611 a.u.

C	1.223467000	1.105309000	-0.395211000
C	2.552791000	0.669671000	-0.234992000
C	1.223874000	-1.105197000	0.395144000
C	2.553033000	-0.669173000	0.234630000
C	0.357496000	-0.000095000	-0.000010000
H	3.435779000	1.254049000	-0.454698000
H	3.436237000	-1.253285000	0.454169000
N	0.814195000	2.299360000	-0.846020000
H	-0.140194000	2.482057000	-1.118473000
H	1.492177000	2.996777000	-1.127094000
N	0.815058000	-2.299370000	0.846016000
H	1.493323000	-2.996596000	1.126883000
H	-0.139192000	-2.482281000	1.118818000
C	-1.839956000	0.963541000	0.683282000
C	-1.840034000	-0.963834000	-0.683164000
N	-2.416112000	1.806812000	1.222238000
N	-2.416529000	-1.806925000	-1.222032000
C	-1.116467000	-0.000249000	0.000160000
H	-2.919553000	2.371524000	1.896059000
H	-2.920085000	-2.371228000	-1.896118000

V-CN'

E = -777.5684008 a.u.

C	-1.76879500	-0.81195300	-0.27653000
C	-2.92322200	-0.02746600	0.27508600
C	-0.96248900	1.13641900	0.42473500
C	-2.44041200	1.13938200	0.69716600
C	-0.56131300	-0.09728500	-0.14593100
H	-3.94747700	-0.37273800	0.29905800
H	-2.98214100	1.96307200	1.14132300
N	-1.95181500	-2.00502000	-0.81549500
H	-1.17709000	-2.51024700	-1.23132300
H	-2.87085700	-2.41751000	-0.89030400
N	-0.22666400	2.19553900	0.68289600
H	-0.64137600	3.03885300	1.05576500
H	0.74826000	2.24309900	0.39182500
C	1.99246400	-1.12125400	0.86190100
C	2.00568100	0.90427200	-0.98942000
N	2.58719100	-1.60402600	1.73052800
N	2.49386900	1.94559900	-1.13346900
Si	1.09807900	-0.74133200	-0.82610900
H	3.12802900	-2.02321200	2.46591000

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V-CN'-T1

E = -777.5227055 a.u.

C	-1.61054400	-0.98730400	-0.22835800
C	-2.81045300	-0.42555900	0.25503100
C	-1.24413800	1.25068200	0.21489500
C	-2.59387800	0.93242000	0.51667500
C	-0.56654700	0.02808700	-0.20109900
H	-3.74443000	-0.95424600	0.38196700
H	-3.32721500	1.63099100	0.89426600
N	-1.43448100	-2.27291400	-0.62223300
H	-0.68621000	-2.51303500	-1.25643200

H	-2.23834400	-2.88281600	-0.66565800
N	-0.69559400	2.46877100	0.33605300
H	-1.25323100	3.24600100	0.65740500
H	0.28533900	2.64594500	0.17061000
C	1.87793500	-1.42212700	0.50978000
C	2.14775500	1.25735600	-0.32856600
N	2.37168500	-2.25904800	1.13396500
N	2.72583100	2.24575300	-0.15505600
Si	1.15592200	-0.23540400	-0.79823300
H	2.80830900	-2.95643800	1.71385200

V-CN''

E = -777.7998139 a.u.

C	-0.60375805	1.61193871	1.08340742
C	-0.06908810	2.90441846	0.55879602
C	0.66790857	1.14564565	-0.70049502
C	0.68762213	2.62705822	-0.50268703
C	-0.13613268	0.51836671	0.28785429
H	-0.28007800	3.87388738	0.98985736
H	1.23096095	3.32148317	-1.12954448
N	-1.38741892	1.59113253	2.13594128
H	-1.64644935	2.44669278	2.61441105
H	-1.76744209	0.73121666	2.51762513
N	1.33951717	0.59552951	-1.68879032
H	1.34610877	-0.40316914	-1.84902256
H	1.88136749	1.15917632	-2.33349978
C	1.03573371	-2.22555372	0.64785012
C	-1.19971744	-1.97435026	-1.01098755
N	1.94294078	-2.87958772	0.92929892
N	-1.81437841	-2.45734313	-1.85887195
Si	-0.63074510	-1.23844954	0.68841972
H	2.72102186	-3.46637634	1.20046713
H	-2.37353771	-2.89384663	-2.58002976

V-CN''-T1

E = -777.7383992 a.u.

C	0.04507100	-1.46960500	1.16138500
C	-0.59610800	-2.64003200	0.70461000
C	0.04507100	-1.46960500	-1.16138500
C	-0.59610800	-2.64003200	-0.70461000
C	0.33380700	-0.63033100	0.00000000
H	-0.98299500	-3.43014000	1.33382300
H	-0.98299500	-3.43014000	-1.33382300
N	0.29488700	-1.15343900	2.44920800
H	1.05009700	-0.53143400	2.70164400
H	0.05690000	-1.82548900	3.16881200
N	0.29488700	-1.15343900	-2.44920800
H	0.05690000	-1.82548900	-3.16881200
H	1.05009700	-0.53143400	-2.70164400
C	-0.17938500	1.93734300	1.36582200
C	-0.17938500	1.93734300	-1.36582200
N	-0.62856600	2.52698900	2.24549700
N	-0.62856600	2.52698900	-2.24549700
Si	0.94747300	1.15007900	0.00000000
H	-1.03944800	3.04642700	3.01230600
H	-1.03944800	3.04642700	-3.01230600