Chemistry–A European Journal

Supporting Information

A Photoionization Study on the Detection of 1-Sila Glycolaldehyde ($HSiOCH_2OH$), 2-Sila Acetic Acid ($H_3SiCOOH$), and 1,2-Disila Acetaldehyde ($HSiOSiH_3$)

Sankhabrata Chandra,[a, b] André K. Eckhardt,[c] Andrew M. Turner,[a, b] György Tarczay,[a, d] and Ralf I. Kaiser*[a, b]

Discussion on Silanes

In this section, TPD profiles of higher silanes are analyzed.[1] Figure S1 shows the PI-ReTOFMS data obtained by photo ionizing the subliming molecules in the TPD phase at photon energies of 10.49 eV, 10.10 eV, 9.92 eV, and 9.60 eV (Table S5). The left column of Figure S1 represents the TPD profile for silanes from disilane (Si_2H_6, 62 amu) to Si_9H_{20} (272 amu). These data are validated through the TPD profiles of the isotopically labelled counterparts. For example, disilane (Si_2H_6, 62 amu) is shifted as D6-disilane (Si_2D_6, 68 amu) by 6 amu. With increasing molecular weight, the sublimation temperature also increases (Figure S2).

Mass to charge ratio *m*/*z* = 60

Isomers of SiH_4CO (60 amu) were also explored. Figure S3a represents the TPD profile for *m*/*z* = 60 recorded at 10.49 eV, 10.10 eV, 9.92 eV, and 9.60 eV with isomers of SiH_4CO represented in Figure S4. The main sublimation observed for *m*/*z* = 60 is due to $Si_2H_4^+$ arising from dissociative photoionization of trisilane (Si_3H_8) at 125 K.[1] The sublimation profile for the SiH_4CO isomer(s) is detected in the 200 K region shown in the inset. At 10.49 eV, 10.10 eV and 9.92 eV, ion counts are observed at 200 K; these TPD profiles are identical after scaling suggesting that a single molecule accounts for these ion counts. However, the ionization energy of **10** is higher than 9.92 eV. Therefore, **10** cannot be ionized, and the ion counts must be linked to isomer **11 - 14**. Upon decreasing the photon energy further to 9.60 eV, signal at *m*/*z* = 60 still remains; at this energy, isomers **11 - 14** can be ionized. At 9.30 eV, we do not observe any ion counts. Therefore, **11** or **12** represents the SiH_4CO isomer. The ionization energies of **11** and **12** are very close and we cannot discriminate between these species. For further validation, TPD profiles are analyzed for the subliming species from the isotopically-substituted SiD_4:CO_2 and SiH_4:$^{18}CO_2$ ices. The sublimation profiles shifted from *m*/*z*=60 for SiH_4:CO_2 ice to *m*/*z*=64 for theSiD_4:CO_2 ice. This confirms that the molecule of interest contains four hydrogen atoms. For the SiH_4:$^{18}CO_2$ ice, the sublimation event shifted by 2 amu to *m*/*z*=62. This confirms that the isomer holds a single oxygen atom. Therefore, mass to charge ratio 60 corresponds to a molecule with the formula SiH_4CO.

VUV generation procedure

Table S3 lists the input parameters utilized to generate a vacuum ultraviolet photon (ω_{vuv}). As an example, the generation of 129.2 nm (9.60 eV) is described here. The 129.2 nm photons were generated by resonant four-wave mixing ($\omega_{vuv}=2\omega_1-\omega_2$) in krypton ($2 \times 10^{-4}$ Torr). For this purpose, 202.3 nm (6.13 eV; ω_1) light was generated from frequency tripling of the dye laser output (606.9 nm; 2.04 eV) using β-BaB_2O_4 (BBO) crystals. The dye laser output 606.9 nm was produced by utilizing a dye laser containing a mixture of Rhodamine 640 and Rhodamine 610 dyes (Exciton), which was pumped by the second harmonic (532 nm; 2.33 eV) of the fundamental of a Nd:YAG laser (1064 nm; 1.17 eV; Spectra Physics, PRO-270-30). The ω_2 component, that is, the 466.7 nm (2.66 eV) light, was produced by using the third harmonic (354.6 nm; 3.49 eV) of the

1064 nm (1.17 eV) fundamental of a Nd:YAG laser (Spectra Physics, PRO-250-30) to pump a dye laser (Sirah, Precision Scan) containing Coumarin 460 dye. In a similar manner other photoionization energies are produced.

References:

1. Tarczay G.; Förstel M.; Maksyutenko P.; Kaiser R. I.; *Inorg. Chem.* 2016, *55*, 8776 – 8785.

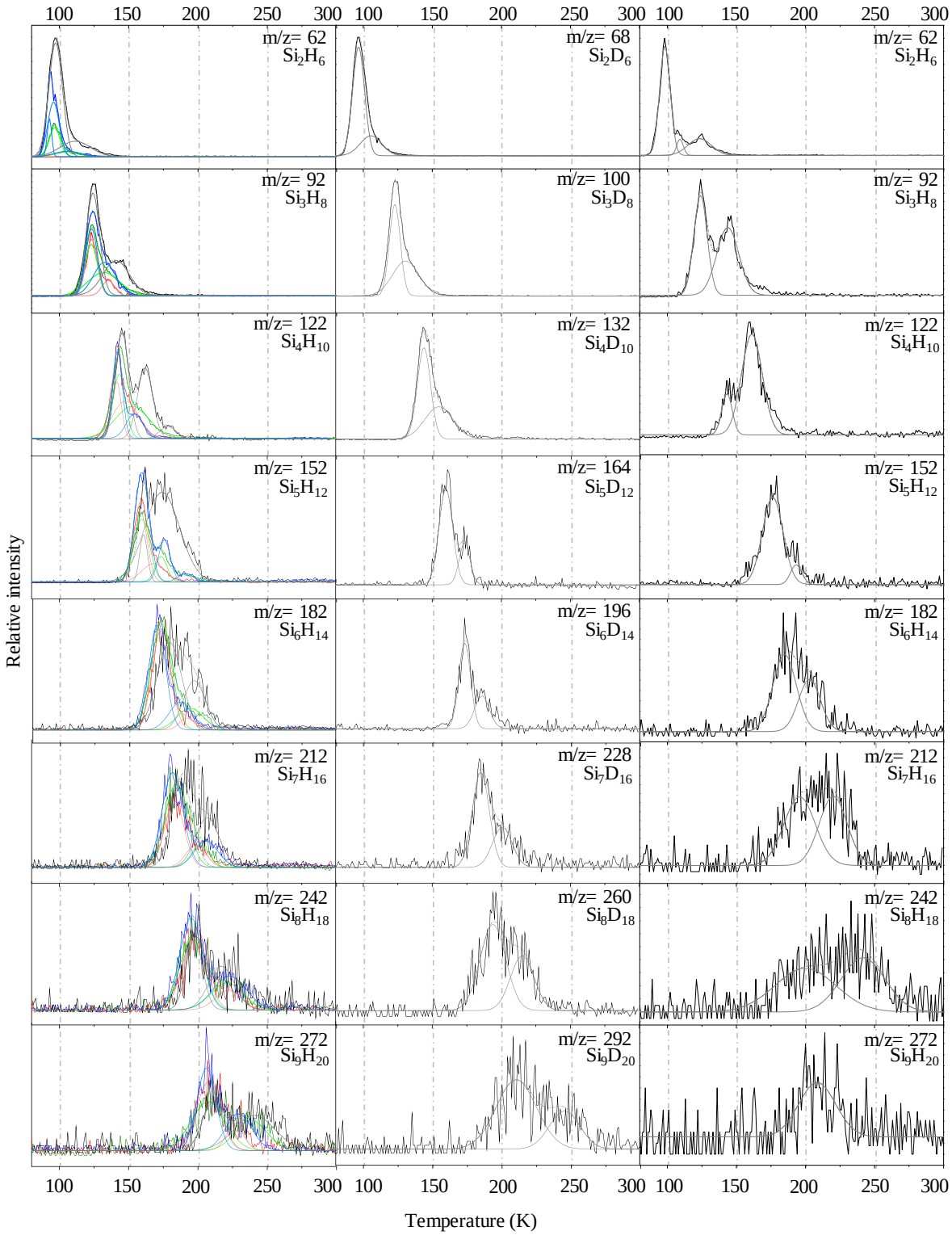

Figure S1: Temperature-programmed desorption profiles of the ionized neutral molecules at distinct mass-to-charge ratios for irradiated SiH_4:CO_2 (left), SiD_4:CO_2 (center), and SiH_4:$C^{18}O_2$ (right) ices. Red: 9.60 eV, green: 9.92 eV, blue: 10.10 eV, black: 10.49 eV

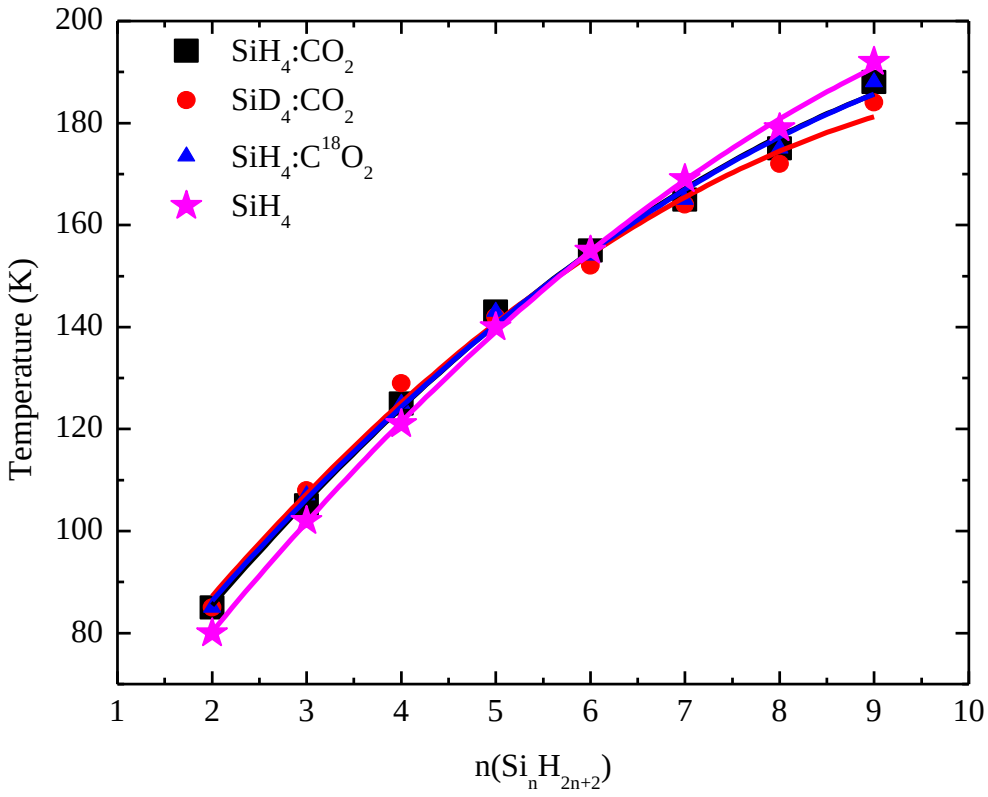

Figure S2: Onset sublimation temperatures for (perdeuterated) silanes observed in irradiated SiH_4:CO_2, SiD_4:CO_2, SiH_4:$C^{18}O_2$, and SiH_4 ices

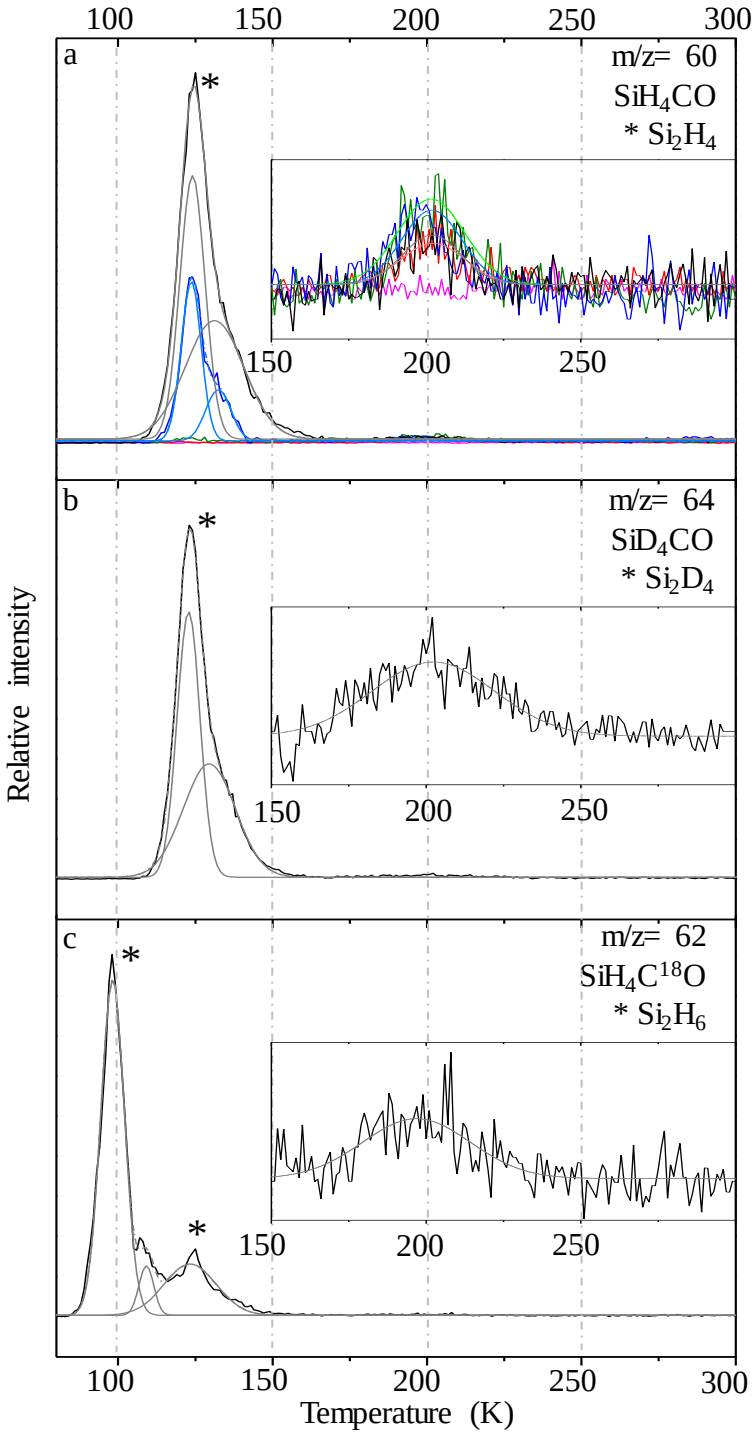

Figure S3: Temperature-programmed desorption profiles of the ionized neutral molecules at distinct mass-to-charge ratios for irradiated SiH_4:CO_2 (left), SiD_4:CO_2 (center), and SiH_4:$C^{18}O_2$ (right) ices. Pink: 9.30 eV, red: 9.60 eV, green: 9.92 eV, blue: 10.10 eV, black: 10.49 eV.

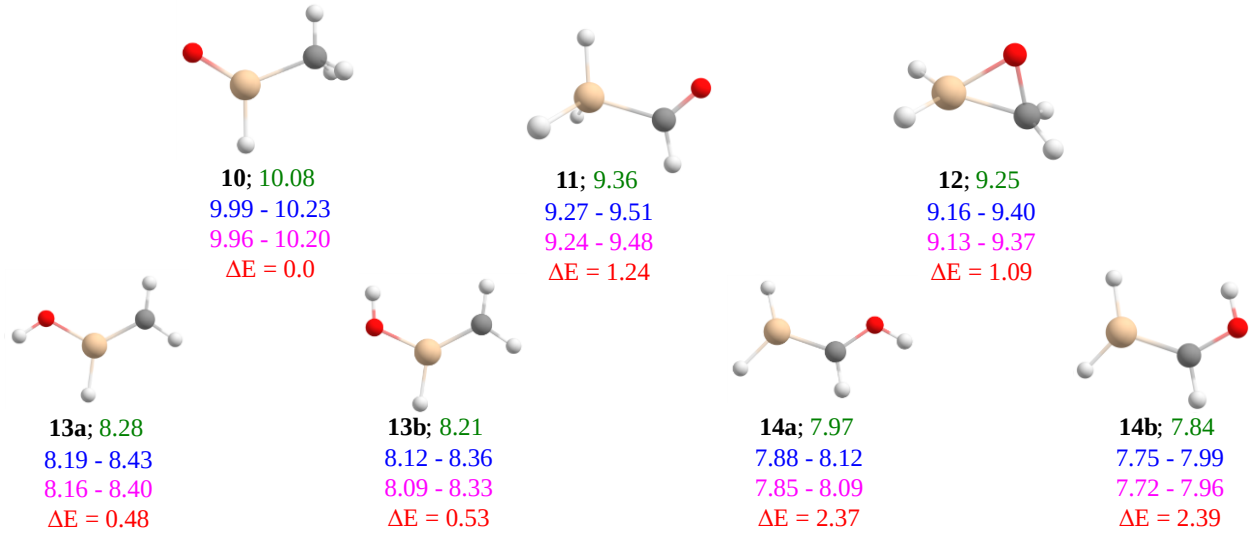

Figure S4: Distinct isomers of SiH_4CO shown in the sequence of decreasing adiabatic ionization energies. Calculated adiabatic ionization energies (green), ionization energy ranges incorporating the error analysis (Table S6) (blue), adiabatic ionization energy ranges corrected for the electric field effect (0.03 eV, pink), and relative energies (red) are shown in eV.

Table S1: Description of different ices with composition, ratio, thickness, irradiation current and time, dose per SiH_4 and CO_2 molecule and used photoionization energy

Ice number	Ice composition	Ice ratio	Ice thickness (nm)	Current (nA)	Irradiation time (s)	Dose (eV SiH_4 $molecule^{-1}$)	Dose (eV CO_2 $molecule^{-1}$)	Photon energy (eV)
I	SiH_4/CO_2	1:1.1±0.1	700±100	21±3	3600±10	1.6±0.2	1.1±0.2	9.60
II	SiH_4/CO_2	1:1.1±0.2	700±100	21±3	3600±10	1.6±0.2	1.1±0.2	9.92
III	SiH_4/CO_2	1:1.1±0.3	700±100	21±3	3600±10	1.6±0.2	1.0±0.2	10.10
IV	SiH_4/CO_2	1:1.2±0.3	700±100	22±3	3600±10	1.7±0.2	1.0±0.2	10.49
V	SiD_4/CO_2	1:1.0±0.2	700±100	22±3	3600±10	1.7±0.2	1.2±0.2	10.49
VI	$SiH_4/C^{18}O_2$	1:1.3±0.3	700±100	21±3	3600±10	1.6±0.2	1.2±0.2	10.49

Table S2: Data applied to calculate the average irradiation dose per molecule.

Initial kinetic energy of the electrons, E_{init} (keV)	5
Average penetration depth, l_{ave} (nm)	350 ± 10
Maximum penetration depth, l_{max} (nm)	550 ± 10
Average kinetic energy of backscattered electrons, E_{bs} (keV)	1.43 ± 0.2
Average kinetic energy of transmitted electrons, E_{trans} (keV)	0
Irradiated area, A (cm^2)	1.0 ± 0.1

Table S3: Parameters used to generate the VUV photons.

YAG 1 wavelength (nm)	Dye 1 wavelength (nm)	Dye 1	YAG 2 wavelength (nm)	Dye 2 wavelength (nm)	Dye 2	Gas, pressure (Torr)	VUV energy (eV)
-	-	-	355	-	-	Xe, 1.3×10^{-4}	10.49
532	606.94	Rh610 / Rh640 mix	532	577.60	Pyrromethene 597	Kr, 1.0×10^{-4}	10.10
532	606.94	Rh610 / Rh640 mix	532	-	-	Kr, 1.0×10^{-4}	9.92
532	606.78	Rh610 / Rh640 mix	355	466.72	Coumarin 460	Kr, 2.0×10^{-4}	9.60
355	445.02	Coumarin 450	532	672.30	Pyridine 1	Xe, 1.5×10^{-4}	9.30

Table S4: Assignments of infrared absorptions of SiH_4:CO_2 ice at 5 K before and after electron irradiation.

Assignments	Positions (cm^{-1})	References
Before irradiation at 5 K		
(CO_2) ν_2	662	1
(SiH_4) ν_4	901	2
(SiH_4) $\nu_2+\nu_4$	1868	2
(SiH_4) ν_3	2174	2
($^{13}CO_2$) ν_3	2277	1
(CO_2) ν_3	2346	1
(CO_2) $\nu_3+\nu_L$	2427	3
(SiH_4) $\nu_3+\nu_4$	3082	2
(SiH_4) $\nu_2+\nu_3$	3142	2
(CO_2)$2\nu_2+\nu_3$	3594	1
(CO_2) $\nu_1+\nu_3$	3701	1
(SiH_4) $\nu_1+\nu_3$	4292	2
New Peaks after irradiation at 5 K		
(Si-H) δ	820-870	4
(SiH_3) ν_4	930	5
(-C=O) ν_1	1700-1750	4
(CO) ν_1	2142	1

[1]C. J. Bennett, C. Jamieson, A. M. Mebel, R. I. Kaiser, *Phys. Chem. Chem. Phys.*, **2004**, *6*, 735
[2]R. I. Kaiser Y. Osamura, *A&A*, **2005**, *432*, 559.
[3]A. M. Turner A. Bergantini, M.J. Abplanalp, C. Zhu, S. Góbi, B. Sun, K. Chao, A. H. H. Chang, C. Meinert, R. I. Kaiser *Nature Comm.* **2018**, *9*, 3851.
[4]Socrates, G., *Infrared and Raman Characteristic Group Frequencies (3rd ed.; New York: Wiley)* **2004**.
[5]L. Andrews , X. Wang, *J. Phys. Chem. A*, **2002**, *106*, 7696.

Table S5: Mass-to-charge ratio of silanes identified in irradiated SiH_4:CO_2, SiD_4:CO_2 and SiH_4:$C^{18}O_2$ ices.

Molecular formula	ǂSiH_4:CO_2	SiD_4:CO_2	SiH_4:$C^{18}O_2$
$^{28}Si_2H_6$	62	68	62
$^{28}Si_3H_8$	92	100	92
$^{28}Si_4H_{10}$	122	132	122
$^{28}Si_5H_{12}$	152	164	152
$^{28}Si_6H_{14}$	182	196	182
$^{28}Si_7H_{16}$	212	228	212
$^{28}Si_8H_{18}$	242	260	242
$^{28}Si_9H_{20}$	272	292	272

ǂ For SiH_4:CO_2, silanes were detected up to Si_{17}.

Table S6: Comparison of experimental to calculated ionization energies of different silicon-containing compounds with average deviations calculated from the error limits. Combined error limits are used to obtain the corrected calculated ionization energies shown in Figure 4 and Figure S4.

Compounds	Experimental IE (eV)	Experimental Error Limits (eV)	References	Computed IE (eV)	Computed IE – Experimental IE (max) (eV)	Computed IE – Experimental IE (min) (eV)
SiH_4	11.1 ± 0.1	11.0 - 11.2	1	10.99	–0.21	–0.01
$(CH_3)_4Si$	9.50 ± 0.03	9.47 - 9.53	2	9.46	–0.07	–0.01
SiO	11.594 ± 0.005	11.589 - 11.599	3	11.61	+0.011	+0.021
SiO_2	12.60 ± 0.05	12.55 - 12.65	4	12.68	+0.03	+0.13
					Average –0.05 ± 0.10	Average +0.03 ± 0.06
					Error Limits –0.15 - +0.05	Error Limits –0.03 - +0.09
					Combined Error Limits –0.15 - +0.09	

1. S.K Shin,. R.R Corderman,. J.L. Beauchamp, , *Int. J. Mass Spectrom. Ion Processes*, **1990**, *101*, 257.

2. M.K. Murphy, J.L. Beauchamp, *J. Am. Chem. Soc.*, **1977**, *99*, 2085.

3. P.R. Stollenwerk, I.O. Antonov, B.C. Odom, *J. Mol. Spec.*, **2019**, *355*, 40.

4. O. Kostko, M. Ahmed, R.B. Metz, *J. Phys. Chem. A*, **2009**, *113*, 1225.

Table S7: Optimized Cartesian coordinates and calculated IR frequencies for the different isomers of SiH_4CO_2

Isomer	Cartesian coordinates				Frequency	Intensity
1	Si	1.575625	–0.219649	0.000000	72.6115	1.1174
	H	1.898889	1.228182	0.000000	122.0313	10.5354
	H	2.102148	–0.871706	1.216103	199.8142	1.8729
	H	2.102148	–0.871706	–1.216103	526.2479	16.8084
	O	–0.097466	–0.405536	0.000000	710.6455	43.2927
	C	–1.049505	0.551174	0.000000	712.5637	27.0148
	O	–2.215569	0.309556	0.000000	889.4571	45.3576
	H	–0.636273	1.573139	0.000000	950.3267	72.3356
					956.1401	277.0845
					968.0051	220.7727
					1041.9827	0.0849
					1176.0245	428.0089
					1416.5487	0.7723
					1835.3338	443.2376
					2229.9451	75.5008
					2262.6111	79.5302
					2267.4098	111.4240
					2963.9466	57.9885
2a	H	1.459633	–1.186660	–0.875029	107.7333	1.8870
	C	1.130601	–0.609349	0.000000	130.3637	24.2234
	O	1.728527	0.675158	0.000000	314.1033	69.4147
	Si	–0.744968	–0.511159	0.000000	448.0144	27.5030
	H	–1.443331	–1.822894	0.000000	448.3490	35.1763
	O	–1.431820	0.855707	0.000000	621.2997	7.7277
	H	1.459633	–1.186660	0.875029	756.1676	25.0112
	H	1.033322	1.345331	0.000000	845.2985	81.4471
					1057.4204	71.3578
					1219.6776	75.7256
					1222.8715	0.0052
					1231.0916	41.7090
					1396.0631	80.5699
					1475.0852	15.6197
					2210.3395	119.2502
					2966.9574	26.0894
					2985.1982	16.0363
					3747.9226	59.3734
2b	H	–0.874071	1.394236	–0.880219	51.8997	24.4126
	C	–0.927560	0.741993	0.000000	191.1626	22.3162
	O	–2.085387	–0.088281	0.000000	231.4476	102.9635
	Si	0.588550	–0.386076	0.000000	336.3449	16.0447
	H	0.194182	–1.816775	0.000000	478.2651	44.1478

	O	2.030675	0.116330	0.000000	676.8482	41.5244
	H	–0.874071	1.394236	0.880219	781.0648	8.0060
	H	–2.871404	0.465730	0.000000	829.4638	85.4580
					1041.0857	63.8487
					1175.4204	49.5625
					1212.6086	1.5368
					1231.7008	60.0389
					1368.0362	20.4341
					1482.0859	9.4754
					2222.6581	98.9648
					2979.0060	27.4138
					3011.4096	15.3356
					3813.2337	41.6949
2c	H	0.944462	–1.377889	–0.729929	51.5072	13.3833
	C	0.957199	–0.638589	0.072740	186.6865	15.1528
	O	2.077362	0.213875	–0.163748	234.3029	135.8288
	Si	–0.681399	0.319313	0.020705	335.0941	15.4744
	H	–0.405083	1.782738	0.059677	455.0468	13.7510
	O	–2.081875	–0.286533	–0.046312	681.9310	27.8155
	H	1.046342	–1.207572	1.004964	752.7963	34.3078
	H	2.246768	0.745135	0.619456	841.4373	59.5814
					1030.7284	82.5423
					1137.0867	30.5692
					1220.6169	85.0726
					1290.9095	8.7409
					1374.4162	26.7357
					1456.7545	6.7704
					2190.2465	122.5278
					2999.6340	19.0992
					3072.4830	3.8642
					3824.5138	40.7332
2d	H	1.436739	–1.159262	–0.877165	103.6442	3.7216
	C	1.159916	–0.552341	0.000000	157.3629	4.4650
	O	1.765377	0.722992	0.000000	266.6755	116.6950
	Si	–0.723553	–0.472051	0.000000	419.4197	73.9009
	H	–1.214562	–1.877809	0.000000	462.2349	31.6880
	O	–1.646009	0.742656	0.000000	598.2270	2.7943
	H	1.436739	–1.159262	0.877165	763.1448	8.4362
	H	2.721306	0.616065	0.000000	866.1137	65.8938
					1079.0990	68.8306
					1188.9826	47.1071
					1220.6386	0.4357
					1241.3446	92.7007
					1378.3309	6.6521
					1475.5266	8.8963
					2194.5105	125.5591

					2930.2076	35.7795
					2953.4045	23.1827
					3809.4034	41.9202
3a	Si	0.303029	–1.332662	0.000000	26.4660	0.1994
	H	–0.360640	–1.856547	1.214064	228.2840	2.0026
	H	–0.360640	–1.856547	–1.214064	399.4718	0.2005
	H	1.741826	–1.677308	0.000000	423.5602	30.9691
	C	0.026229	0.579419	0.000000	628.9615	55.4992
	O	1.164799	1.315028	0.000000	655.5580	144.5232
	O	–1.069133	1.081231	0.000000	692.9788	26.3190
	H	0.900792	2.251446	0.000000	743.0262	5.1373
					909.9498	228.1552
					943.6352	38.7499
					949.0417	47.4968
					1126.1944	225.1522
					1309.2541	7.7605
					1773.9886	246.3278
					2242.9835	38.3177
					2257.1094	85.4338
					2258.1687	95.7443
					3671.0345	35.7924
3b	Si	0.272497	–1.313981	0.000000	77.5302	0.0020
	H	–0.365752	–1.853919	1.219012	224.6123	13.4389
	H	–0.365752	–1.853919	–1.219012	397.5453	64.7883
	H	1.724002	–1.637429	0.000000	416.5427	9.9762
	C	0.006258	0.604203	0.000000	534.4034	26.7591
	O	1.083764	1.439740	0.000000	633.3501	39.1405
	O	–1.102962	1.060437	0.000000	715.8404	25.6685
	H	1.901912	0.928449	0.000000	719.0728	14.6234
					909.0513	235.8396
					943.6523	44.8056
					945.5362	47.1165
					1115.1984	30.9256
					1270.7453	346.1518
					1803.8744	205.5781
					2207.0791	94.8434
					2255.4237	51.7354
					2265.4564	76.7993
					3786.8182	46.2518
4a	H	2.223685	–0.620054	0.000000	120.2070	0.4073
	C	1.112214	–0.660013	0.000000	158.7111	21.5943
	Si	0.000000	0.921750	0.000000	343.9341	83.8892
	H	0.286959	1.734017	1.208045	423.8890	28.6568
	H	0.286959	1.734017	–1.208045	467.4405	36.4624
	O	–1.543984	0.343659	0.000000	619.5681	29.5370
	O	0.558240	–1.740159	0.000000	719.4804	13.0723

	H	–1.584939	–0.620406	0.000000	813.3680	54.1761
					909.1038	118.4791
					912.5321	25.2276
					960.8795	227.2371
					978.4504	109.9903
					1385.1672	12.5354
					1727.0897	108.8612
					2221.0294	136.6307
					2222.1200	82.4109
					2831.3947	153.4382
					3795.4964	89.7721
4b	H	–0.452580	–1.892929	0.000000	67.1638	10.1047
	C	0.385383	–1.158416	0.000000	158.1648	9.4695
	Si	0.000000	0.729369	0.000000	168.4305	105.9926
	H	0.608981	1.339836	1.208703	344.0035	1.0996
	H	0.608981	1.339836	–1.208703	495.5016	30.5732
	O	–1.654895	0.832668	0.000000	684.9867	17.6447
	O	1.530175	–1.550088	0.000000	710.3058	36.3686
	H	–2.079927	1.691944	0.000000	788.7616	228.1184
					847.5183	44.5401
					902.3558	21.9017
					940.8693	179.0305
					975.1234	97.0744
					1382.9251	16.3351
					1745.5564	108.5061
					2215.0359	84.0602
					2217.7967	145.0292
					2810.9506	143.1685
					3889.2323	93.3620
4c	H	2.207176	–0.550861	0.000000	72.6652	19.9596
	C	1.100687	–0.712928	0.000000	130.9082	97.1005
	Si	0.000000	0.869883	0.000000	146.3369	2.7784
	H	0.356871	1.670101	1.203123	429.0220	30.6613
	H	0.356871	1.670101	–1.203123	457.8741	22.4666
	O	–1.572709	0.374239	0.000000	592.1642	59.6119
	O	0.666196	–1.839107	0.000000	714.1404	38.1850
	H	–2.272931	1.028806	0.000000	784.7506	181.9061
					856.9952	33.9481
					915.2573	21.0178
					954.0057	145.2623
					980.5363	120.9757
					1397.4026	13.4028
					1756.8101	125.3937
					2195.3622	154.2757
					2196.3451	89.3440
					2765.1283	174.0625

					3894.8505	106.7813
4d	H	–0.312203	–2.008919	–0.237766	49.9458	9.5698
	C	0.450495	–1.216435	–0.049101	157.6545	11.6572
	Si	–0.053435	0.650937	–0.004736	200.7627	110.3380
	H	0.514757	1.218558	1.243450	335.6447	3.0106
	H	0.530924	1.297717	–1.198994	471.7867	25.5655
	O	–1.694903	0.864191	–0.106909	684.2391	1.0383
	O	1.608339	–1.529516	0.113848	702.0648	52.2233
	H	–2.226385	0.768267	0.685312	830.1033	125.9484
					881.5154	199.3026
					893.2478	49.4149
					918.6816	90.6162
					949.1866	81.1803
					1383.5537	14.5621
					1742.4240	95.7359
					2219.5908	101.2358
					2253.7592	94.5090
					2790.0060	169.7603
					3888.9733	96.4436
5a	Si	–1.453025	0.165652	0.000000	195.3257	6.8179
	H	–1.734081	–0.723151	–1.183588	269.2828	17.7007
	H	–1.734081	–0.723151	1.183588	395.3267	42.4964
	C	0.409293	–0.089123	–0.000000	452.9265	12.0188
	O	1.186691	–0.058573	–1.071228	552.0315	0.1123
	O	1.186691	–0.058573	1.071228	610.3736	91.0735
	H	0.631534	–0.115899	–1.859404	659.7402	79.5336
	H	0.631534	–0.115899	1.859404	707.1731	7.3603
					720.4521	32.3669
					946.4977	113.2005
					1148.6671	54.2422
					1180.2959	393.4326
					1416.6893	19.9314
					1437.1055	615.1069
					2089.3789	99.7760
					2104.8496	193.6784
					3781.8319	177.2115
					3783.0230	6.8099
5b	Si	–1.445318	–0.051585	–0.128037	230.2763	11.3761
	H	–1.794010	–1.169335	0.802161	278.9708	9.0929
	H	–1.697174	1.210757	0.656807	382.5658	48.4187
	C	0.408088	–0.025602	0.062406	443.2602	28.1520
	O	1.169110	–1.104464	0.008916	518.5240	175.2638
	O	1.155110	1.083037	–0.012052	570.6427	18.9094
	H	2.099614	–0.850634	–0.100632	640.2042	39.4809
	H	0.583735	1.856434	0.084830	682.7094	40.0600
					712.2155	22.1130

					947.0249	135.7587
					1111.9428	236.0972
					1198.4696	183.6952
					1363.4868	177.8274
					1464.0780	349.9758
					2090.0159	147.8372
					2158.0108	121.4043
					3698.1777	107.3129
					3768.7062	80.7718
5c	Si	–1.425755	–0.012349	–0.109861	183.4243	213.9851
	H	–1.927319	–1.165199	0.682317	258.2525	74.2275
	H	–1.886978	1.282284	0.454178	302.2192	147.3692
	C	0.377085	–0.002683	0.076120	368.7103	34.2586
	O	1.105589	–1.134721	–0.045827	445.1726	48.0873
	O	1.097977	1.136924	0.065125	516.5416	23.3283
	H	2.001617	–0.995798	0.290062	552.2395	16.3215
	H	1.882222	1.050073	–0.499601	672.4695	45.5611
					695.9717	1.9485
					928.1608	135.7264
					1097.8464	295.6363
					1181.4334	22.8822
					1258.0199	306.7505
					1446.1034	106.8990
					2195.6353	59.2268
					2221.3473	113.5378
					3669.3769	17.3392
					3746.6021	86.7387
6a	H	0.917542	1.575631	–0.064110	95.9235	47.7854
	C	0.939011	0.497081	0.055697	168.6040	11.6670
	O	2.231004	0.049576	0.003947	190.9523	59.7702
	Si	–0.548934	–0.410130	–0.127936	335.6628	47.1386
	H	–0.567858	–1.810805	0.342329	397.5742	9.3322
	O	–2.004123	0.328536	0.180343	429.5593	42.6634
	H	2.266206	–0.885946	0.231086	746.1715	52.2829
	H	–2.379927	0.855554	–0.526705	781.4650	37.9120
					850.8724	57.8261
					881.8312	314.9279
					923.6719	9.1423
					1164.7262	248.6969
					1262.1009	38.6782
					1435.4282	68.2605
					2249.5027	66.6659
					3139.1373	6.7482
					3789.6915	53.0155
					3888.5289	139.9376
6b	H	0.917344	1.575534	–0.064092	92.3790	48.5656

	C	0.938967	0.496987	0.055740	168.5809	11.6438
	O	2.230988	0.049694	0.003897	190.7036	58.9699
	Si	–0.548925	–0.410255	–0.127893	335.6567	47.2227
	H	–0.567828	–1.810836	0.342698	397.5528	9.2818
	O	–2.004099	0.328901	0.180446	429.4133	42.6757
	H	2.266257	–0.885862	0.230859	745.9251	52.7808
	H	–2.379741	0.854048	–0.528137	781.3861	37.9427
					850.6962	59.0208
					881.5872	312.0545
					923.6433	10.3984
					1164.6625	248.7062
					1262.0048	38.6103
					1435.3696	68.2010
					2249.5908	66.6253
					3139.1543	6.7540
					3789.6040	52.9951
					3889.1291	140.0660
6c	H	1.625933	–1.426990	0.050319	97.2524	2.2340
	C	1.064098	–0.498588	0.089023	203.3570	67.2164
	O	1.894940	0.568626	–0.033242	271.8451	131.1236
	Si	–0.679257	–0.572957	–0.116179	356.4447	37.2050
	H	–1.305841	–1.725229	0.567140	492.0757	22.7991
	O	–1.460369	0.881622	0.148623	518.9180	43.0130
	H	1.388594	1.380926	0.087740	705.4493	36.2031
	H	–2.060254	1.182230	–0.535874	775.3591	53.4752
					803.9112	70.6275
					867.7278	173.6540
					917.5630	42.6579
					1173.1969	275.4854
					1286.2970	51.3717
					1444.5413	113.6326
					2238.9998	72.9616
					3139.6344	5.7433
					3771.9662	63.6157
					3886.9222	145.4385
6d	H	1.576355	–1.455268	0.031462	119.3446	1.3524
	C	1.055580	–0.501907	0.059066	173.9339	57.8855
	O	1.841634	0.638763	0.059972	243.6325	97.6015
	Si	–0.664386	–0.523573	–0.059683	293.9320	128.5485
	H	–1.422104	–1.745505	0.232100	421.7664	13.8936
	O	–1.663316	0.787738	0.030766	456.3931	69.6537
	H	2.640145	0.477996	–0.452034	660.7036	18.5629
	H	–1.253015	1.652229	–0.056266	733.2892	13.0153
					780.5024	72.9465
					906.1853	103.2587
					959.4520	166.9358

					1160.9824	186.7171
					1203.7577	40.9350
					1439.2307	10.4747
					2313.7625	43.2304
					3113.8412	11.2340
					3796.0776	64.6708
					3863.6886	98.1695
6e	H	0.944914	1.592505	–0.030627	136.1514	48.9831
	C	0.932389	0.506780	0.025141	167.5550	41.7560
	O	2.172698	–0.118728	0.107149	183.8241	11.7118
	Si	–0.536662	–0.389775	–0.063757	309.5229	191.5709
	H	–0.649330	–1.843092	0.106087	355.9106	5.5034
	O	–2.046352	0.270624	0.055076	378.1404	30.7479
	H	2.749643	0.231454	–0.579575	734.8552	26.9357
	H	–2.137065	1.220148	–0.051940	746.0845	64.3428
					836.7147	100.8125
					900.1745	93.6489
					939.2718	167.0937
					1134.0490	118.9159
					1213.7705	22.0918
					1417.2583	10.8254
					2312.8433	41.9180
					3098.7008	20.0917
					3775.4884	48.8923
					3876.5242	96.9605

Table S8: Optimized Cartesian coordinates and calculated IR frequencies for the different isomers of Si_2H_4O

Isomer	Cartesian coordinates				Frequency	Intensity
7	Si	1.577541	–0.192680	0.000000	47.1351	4.3433
	H	2.072800	–0.903463	1.206348	182.0405	24.9159
	H	2.072800	–0.903463	–1.206348	382.3329	30.0718
	H	2.035094	1.213920	0.000000	390.9727	6.5679
	Si	–0.786029	–0.275936	0.000000	525.7647	18.0270
	H	–1.349901	–1.660600	0.000000	561.1607	1.0284
	O	–1.688830	0.961660	0.000000	827.7177	276.4745
					878.9814	64.5871
					938.4936	39.4302
					939.8044	36.5687
					1204.1719	67.1357
					2153.5621	159.1921
					2212.0985	41.2259
					2222.0869	72.5453

					2255.3996	62.5651
8	Si	0.000000	1.104377	–0.252708	392.8130	6.2208
	H	–1.216064	1.946720	–0.333426	486.2387	7.7776
	H	1.216064	1.946720	–0.333426	518.7664	15.1262
	Si	–0.000000	–1.104377	–0.252708	524.1537	0.0000
	H	–1.216064	–1.946720	–0.333426	634.3653	0.0000
	H	1.216064	–1.946720	–0.333426	666.9223	49.6424
	O	–0.000000	0.000000	1.051192	761.8229	4.9125
					777.5022	196.1815
					896.5725	172.6872
					973.7534	215.8492
					975.2194	21.1616
					2217.4649	181.4381
					2224.9448	3.0234
					2233.1681	0.0000
					2240.8853	224.2839
9a	Si	1.559024	–0.180178	–0.131321	162.7240	12.2803
	H	2.329997	0.885513	0.579394	252.6637	14.0546
	H	1.733530	–1.449277	0.640639	311.7106	35.7620
	Si	–0.560236	0.468801	0.099487	394.4214	32.0844
	H	–1.030253	1.805610	–0.344148	455.3213	32.3950
	O	–1.899991	–0.484042	–0.074784	537.6852	6.7954
	H	–1.816386	–1.410230	0.168061	573.7385	7.2488
					794.2080	61.3114
					887.6654	360.0943
					925.7635	48.0337
					938.2310	50.4885
					2147.1262	90.4568
					2169.3554	91.9590
					2218.6530	118.3645
					3857.9420	119.2451
9b	Si	–1.563650	–0.176269	0.135040	165.4688	1.0288
	H	–2.324819	0.934501	–0.514367	258.8950	58.6856
	H	–1.820798	–1.424049	–0.641863	287.6452	86.8812
	Si	0.555089	0.447749	–0.108274	385.6513	18.2348
	H	1.002556	1.783364	0.387844	442.8014	23.5603
	O	1.827314	–0.600516	–0.000501	522.1119	10.4558
	H	2.644400	–0.290397	0.397660	557.9586	22.4735
					766.8233	168.3963
					851.3559	112.8581
					930.6426	139.8516
					962.8842	55.9935
					2154.7320	108.2713
					2167.8548	56.8621
					2182.9994	154.9315
					3862.8562	145.5416

Table S9: Optimized Cartesian coordinates and calculated IR frequencies for the different isomers of SiH_4CO

Isomer	Cartesian coordinates				Frequency	Intensity
10	C	–1.647244	–0.165335	0.000000	91.7624	1.6562
	Si	0.139801	0.356952	0.000000	274.4725	24.5244
	H	0.268059	1.838895	0.000000	486.6638	20.4194
	O	1.355630	–0.567911	0.000000	658.6767	1.8516
	H	–2.154112	0.241607	–0.878456	760.6107	77.7119
	H	–2.154112	0.241607	0.878456	774.0461	30.8019
	H	–1.742047	–1.249231	0.000000	926.2756	44.7467
					1229.8592	88.1223
					1284.3495	41.3430
					1445.7478	3.7279
					1450.1518	5.7893
					2201.1715	127.9138
					3023.7143	0.3523
					3084.4579	2.1239
					3132.3000	0.9008
11	Si	0.485564	–0.945615	0.000000	70.1911	4.9838
	H	–0.116163	–1.571705	1.204899	284.6532	15.9272
	H	–0.116163	–1.571705	–1.204899	480.7133	16.2532
	H	1.956606	–1.096117	0.000000	530.286	17.2167
	C	0.023353	0.935405	0.000000	735.4116	37.3054
	O	0.848516	1.817338	0.000000	904.7323	180.4035
	H	–1.060530	1.201435	0.000000	905.2691	47.2165
					943.8402	41.3239
					945.7493	17.8629
					1395.5307	20.7174
					1748.224	138.1036
					2215.0407	47.0121
					2222.825	101.4838
					2259.3393	79.5718
					2786.7174	159.9783
12	C	0.705363	–0.905094	0.000000	492.2313	2.2075
	Si	0.000000	0.768780	0.000000	604.7016	1.5655
	H	–0.101390	1.579629	1.229909	641.0222	31.2145
	H	–0.101390	1.579629	–1.229909	736.0251	38.7565
	O	–0.771153	–0.717984	0.000000	769.5603	102.2696
	H	1.069914	–1.373872	0.908737	815.6800	35.7960
	H	1.069914	–1.373872	–0.908737	946.4776	41.2802
					1025.9265	81.5783
					1107.7842	1.6988
					1129.1288	2.3621
					1471.5915	1.4938
					2251.6245	59.7772
					2267.3450	119.6875

					3078.9425	23.3078
					3155.7409	10.9631
13a	C	–1.566087	–0.398222	0.000000	264.5116	19.4768
	Si	–0.057405	0.377774	0.000000	299.1450	124.4899
	H	0.153454	1.830725	0.000000	377.0107	3.7248
	O	1.435326	–0.317121	0.000000	584.4909	3.2130
	H	–2.465777	0.202513	0.000000	651.2779	20.2785
	H	–1.709844	–1.469116	0.000000	705.6790	42.4583
	H	1.483201	–1.276513	0.000000	797.6625	115.0273
					885.5923	78.3691
					916.4433	39.6929
					1053.1123	124.9479
					1381.7061	18.5898
					2312.1424	49.7239
					3146.6247	0.1546
					3233.7884	0.2205
					3866.8873	98.2787
13b	C	1.560379	0.394237	0.000000	182.3460	91.9329
	Si	0.055620	–0.383108	0.000000	262.6665	3.6403
	H	–0.130473	–1.847083	0.000000	365.2133	21.4289
	O	–1.383477	0.417889	0.000000	584.6138	26.1044
	H	2.459622	–0.206154	0.000000	647.0253	34.7794
	H	1.692591	1.465840	0.000000	709.3393	37.3287
	H	–2.188109	–0.103932	0.000000	825.3870	36.6706
					841.9898	218.3095
					904.2877	13.7620
					1071.5910	88.1255
					1380.3298	18.4356
					2265.7602	68.7465
					3153.3665	0.0327
					3244.7329	0.0050
					3890.1070	135.0044
14a	Si	–1.117782	–0.090392	–0.061014	225.0634	64.7076
	H	–1.377533	–1.512801	0.255318	282.0637	19.2484
	H	–2.149621	0.884592	0.335635	440.5715	28.8351
	C	0.532211	0.487153	0.047377	493.1497	32.2987
	O	1.712956	–0.182164	–0.013326	632.5839	27.6007
	H	0.713135	1.555436	–0.018365	807.2978	17.4303
	H	1.566054	–1.127340	0.103962	847.0519	39.0008
					924.8058	50.5126
					1178.9610	304.6800
					1281.5618	60.6090
					1446.9430	106.6702
					2235.2813	41.4998
					2280.7459	67.0516
					3140.5174	4.3008

					3787.7094	57.8066
14b	Si	–1.124274	–0.082662	–0.044661	195.7959	44.6472
	H	–1.497257	–1.493542	0.163474	278.1863	13.9989
	H	–2.142817	0.947447	0.221516	328.7598	97.6133
	C	0.527548	0.456826	0.036323	473.4626	12.6091
	O	1.634983	–0.342893	0.026498	625.9324	54.6668
	H	0.719862	1.526115	–0.007608	777.3021	20.3670
	H	2.414900	0.179437	–0.182044	834.4092	19.3813
					920.7243	40.9756
					1187.0491	345.2881
					1227.5553	25.3017
					1469.7120	37.4967
					2263.8214	22.0083
					2294.2786	71.8969
					3109.4498	10.8227
					3817.2930	112.7200