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date: July 20, 2022

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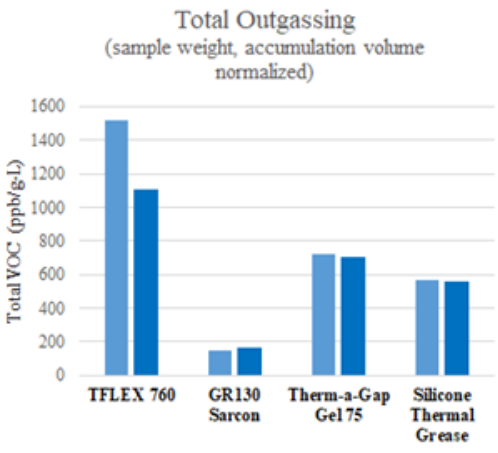
subject: *Cryo-GCMS Outgassing Screening: Thermal Filler Materials*

Executive Summary

A study was conducted to investigate the outgassing characteristics of four thermal filler materials (see Table I). The purpose of this screening was to identify any outgassing products that might be considered reactive, specifically compounds that could result in corrosion in the systems where these materials are used. A range of compounds was observed in the sample headspaces, though most do not stand out as being known reactive species of concern. However, several halogenated compounds and sulfurous compounds- classes compounds known to facilitate corrosion reactions under certain conditions- were observed in low concentrations. The *TFLEX 760* exhibited the highest total outgassing, while the *GR130* had the lowest. *Therm-a-Gap75* and the *Si thermal grease* exhibited very similar outgassing profiles. It is difficult to predict the extent to which any given compound observed in an analysis of this type might pose a risk in an actual system; factors such as temperature, system geometry, concentration, and gas conductance all play a role in the kinetics governing chemical reactions. It is recommended that the results of these analyses are shared with pertinent materials SMEs familiar with the system(s) in question to evaluate potential risks. A summary of the results is presented below in Table I.

Table I. Summary of outgassing screening of 4 thermal filler materials via cryofocusing GC/MS: duplicate samples of each material held under dry N_2 (100 cc) @ 80 °C for ~48 hours; cooled to RT before performing headspace analysis. "Total outgassing" is the sum of all estimated peak concentrations in each sample headspace, normalized to sample mass and 1L accumulation volume to provide an approximate relative measure of how extensively each material outgassed in ppb/g-L.

MATERIAL(S):	weight (g)	total VOC (ppb)	sulfur compounds (ppb)	halogenated compounds (ppb)
TFLEX 760	1.07	16194	0.0	372.8
	1.07	11841	0.0	3.7
GR130 Sarcon	0.70	1063	0.0	1.4
	0.61	1020	0.0	1.6
Therm-a-Gap Gel 75	0.72	5174	47.1	39.0
	0.74	5238	53.2	20.1
Silicone Thermal Grease	0.55	3131	0.0	31.1
	0.55	3057	0.0	31.2
(blank)	--	23	0.0	0.0



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Background

Reactive outgassing compounds, even in low concentrations, can have the potential to facilitate undesirable chemical reactions in certain systems.[1] Several recent studies have revealed that low-molecular weight sulfurous compounds of concern from a corrosion standpoint (e.g., *carbonyl sulfide*) can evolve from materials that contain ostensibly stable, higher molecular-weight sulfur-containing species through as-yet unknown chemical mechanisms.[2-7] The source of the corrosive sulfur outgassing products in these in materials may be endemic to the material itself (like PPS, which consists of aromatic rings linked by thioether groups) or exist as contamination (as seems to be the case with certain PAEK polymers, which have been found to contain residual diphenyl sulfone used in the synthesis process). Thus, it is not necessarily sufficient to simply evaluate the chemical structure or composition of a given material as a basis for predicting its outgassing properties, as the origins of certain compounds entrained in the material appear to be more nuanced than previously assumed. Instead, testing is needed to directly evaluate the outgassing characteristics of a given material.

The aim of this study was to determine the general outgassing profile of the materials provided and to identify any VOCs (volatile organic compounds) of potential concern from an aging & lifetime / materials compatibility standpoint, particularly those that could contribute to degradative reactions of the parts with which the material will be in close contact (e.g., sulfur containing compounds, acids, etc.).

Experimental – Outgassing Screening

The four materials underwent testing in duplicate in this study (see Table I). The samples were sealed in stainless-steel headspace vials (~100 cc, verified clean) using gold-plated Cu gaskets, evacuated and backfilled with dry N_2, and held at 80 ºC for ~48 hours to increase the rate of outgassing from the material and the accumulation of gas-phase outgassing products in the headspace. The sample headspaces were then analyzed via cryo-GC/MS according to the parameters outlined below in Table II.

A 200 ppb VOC standard mix (Ozone Precursor) was analyzed at the same volume and pressure as the samples and was used to determine an average compound response factor under the known sample conditions. This was applied to the observed compound peak areas in the sample TICs (Total Ion Chromatograms), yielding a semi-quantitative estimation of concentration for each observed compound.

Table II. Outgassing screening analysis parameters.

Preconcentration Parameters	
Instrument:	Entech 7200 cryofocusing preconcentrator
Injection Volume:	20 cc
Method:	"Sandia-001.ctd3"
GC (Gas Chromatography) Parameters	
Instrument:	Thermo Trace 1310
Column:	Thermo-Scientific DB5 (60m x 0.32mmID x 1µm)
Method:	"-20-230-DB5"
Column Flow:	Constant, 1.5 mL/min

Method Parameters:	**Temp (°C)**	**Time (min)**	**Rate (°C/min)**
inject & hold:	-20	1	--
ramp to:	230	27	10
hold:	230	1	

total run time:	29

Detector Parameters:

Type:	Mass Spectrometer
Instrument:	Thermo ISQ 7000
Mass Range:	30-300 m/z
Dwell Time:	0.2 seconds

A Note on Cryofocusing Gas Chromatography / Mass Spectrometry

In GC/MS, a Total Ion Chromatogram (TIC) is generated for each sample, which is a plot of the mass spectrometer detector response intensity vs. time. In these plots, each peak represents a unique chemical compound that was present in the gas sample and separated in the GC column. Cryo GC/MS can be generally described as follows: volatile and semi-volatile organic compounds (VOCs) that outgas from materials in a closed vessel accumulate in the gaseous headspace of the vessel. These VOCs are pre-concentrated from a gas sample by condensing them onto a cryogenically cooled surface. Permanent gases (N_2, O_2, Ar, etc.) invariably make up the bulk of the gas sample. These permanent gases (not of interest in this investigation) have freezing points much lower than the volatile compounds and therefore do not condense with the VOCs. The non-condensed permanent gases are flushed from the sample, leaving only the "frozen" VOCs on the cold surface. This concentrated VOC mix is then quickly heated and injected into the GC column and separated into its individual constituents. As the individual chemical compounds from the pre-concentrated mix elute from the GC column, they are ionized by the mass spectrometer and directed to a detector (electron multiplier) which generates an electrical current. This current is proportional to the amount of that particular chemical compound present in the original sample.

Major peaks in this analysis are identified using an automated search routine with a cursory manual verification. Peaks in each TIC were manually selected for integration. Peak identifications are based on a best match from NIST library database, which was done using Thermo-Scientific Chromeleon (version 7.2 SR4) software and with automated mass spectral deconvolution and identification system (AMDIS version 2.72). Sample headspaces were compared directly with reference gas standard containing a mix of ~50 organic (hydrocarbon) compounds, each in a concentration of 200 ppb. Semi-quantitative estimations of compounds observed in the sample headspaces were made in reference to the average 400 ppb response factor from the VOC standard. While the automated peak identification routine used in this analysis is generally very accurate, the identifications herein (especially those of very low-abundance compounds) should be considered tentative without further verification and/or corroborating analysis.

This type of analysis is intended to provide a general summary of the major VOC components present in the sample headspace gas and a first-order approximation of their respective contributions to the overall VOC profile. It should be understood that conclusions about the absolute amount of a compound that can be expected to exist in the system in which the sample material is used cannot be drawn from this analysis alone. This analytical technique can very useful as an initial screening to identify VOC products that may be of concern in a particular system or application. However, without rigorous analyses to quantitate these compounds and the extent to which they persist in the long-term outgassing profiles of the materials, it is generally not possible to draw conclusions about the amounts of these compounds that could be expected to accumulate in an actual system or component.

Results

Under the conditions of this study, cryo-GC/MS analysis of the sample headspaces yielded chromatograms with all peaks on scale and with repeatable results between duplicate samples. However, two compounds (*trimethylsilyl fluoride* and a complex *trisiloxane* compound) appeared in relatively high concentrations in one of the TFLEX samples but not the other; this reason for this discrepancy is not known. This can be seen below in Figure 1, which plots the total ion chromatograms (TICs) for all the samples, the blank, and the 200 ppb VOC standard.

Total outgassing: comparison

Not all sample weights were identical in this study, so the estimated raw concentrations measured in the sample headspaces cannot strictly be used to compare the total outgassing of the four materials. However, the measured concentrations can be normalized to the sample weights and accumulation volumes to provide a basis for direct comparison. (This assumes a direct proportional relationship between total outgassing accumulation and sample amount. In reality, the dynamics that dictate outgassing rates and accumulation concentrations are far more nuanced, exhibiting dependence on a number of other factors such as sample geometry, analyte concentration in headspace and in material, etc. However, this approach is considered a good first-order means by which the relative total "amount" of outgassing between materials can be gauged.) This is illustrated in Table I, where the total estimated concentration of all VOCs detected in the analysis are normalized to the sample weight (per gram basis), as well as an accumulation volume of 1 L. Thus, the "Total VOC" count displayed in that table can be interpreted as "the approximate total concentration (in parts per billion) of volatile organic compounds (VOCs) that will accumulate in a 1L volume headspace from 1 gram of material under the time/temperature conditions of this study."

Observed compounds: comparison

The same normalization approach was administered to the highest abundance individual compounds detected in this study, presented in Figure 2. In this plot, it can clearly be seen that the "*TFLEX 760*" (blue) samples outgassed significantly more compounds than the other samples. Conversely, the *GR130 Sarcon* samples (orange) contribute far less to this suite of observed compounds. The similarities between *Therm-a-Gap 75* (green) and the *silicone thermal grease* (red) are also evident, illustrated by the frequent coappearance of red and green peaks in similar concentrations.

Full inventory of observed compounds

A full reporting of the observed gas-phase compounds observed in each of the sample headspaces is presented in Appendix A and Appendix B. However, it should be noted that the estimated concentrations reported in Appendix A and Appendix B are the *raw* compound concentrations, not normalized.

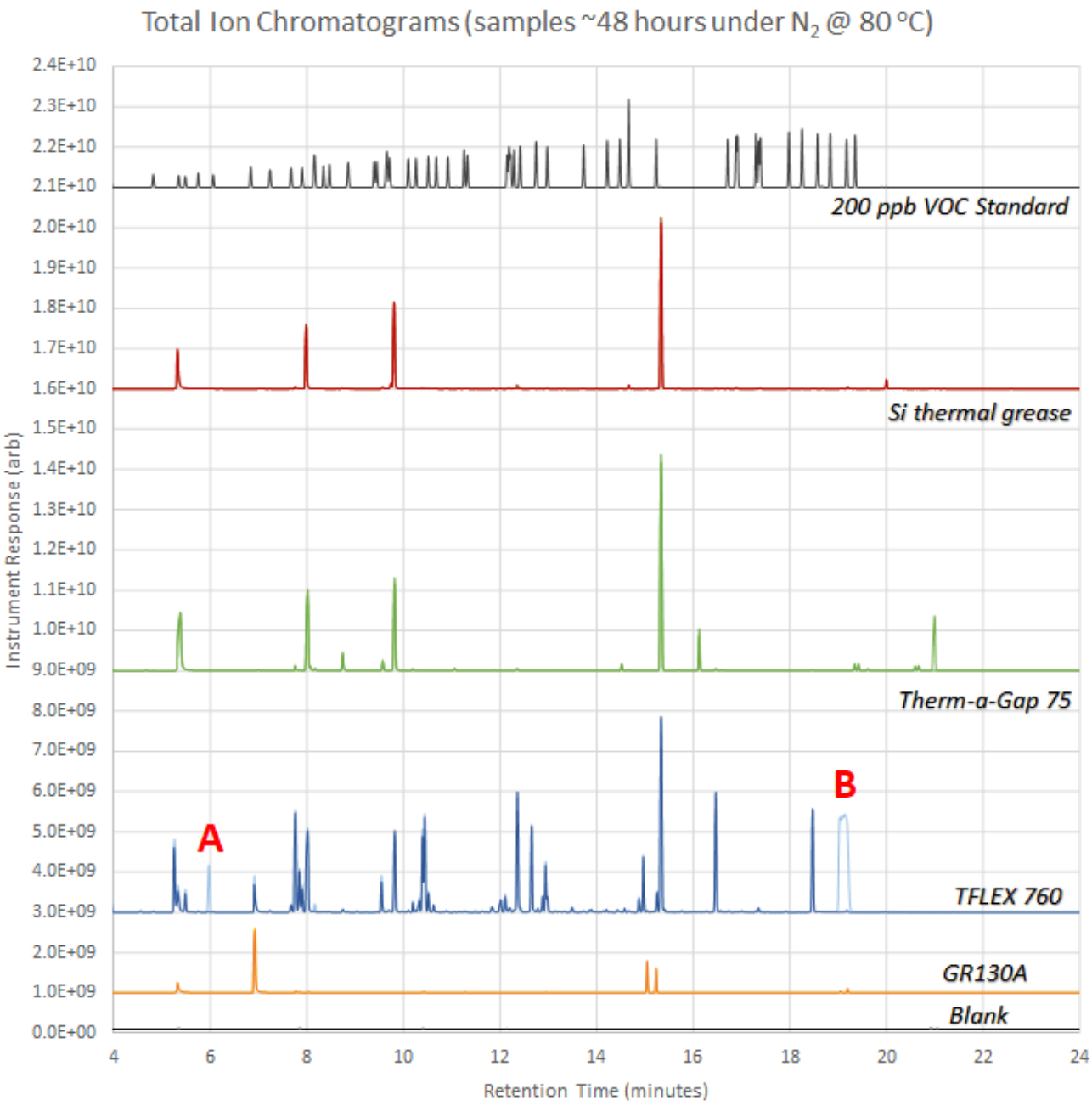

Figure 1. Total Ion Chromatogram (TIC): cryo-GC/MS headspace analysis of 4 thermal filler materials held at 80 C for ~48 hours under N_2, along with blank vial and 200 ppm VOC standard gas mix. Each peak corresponds to a unique compound detected in the analysis. TICs are plotted on same intensity scale and offset for clarity. Two compounds appeared in one of the TFLEX 760 samples but not the other; A) trimethylsilyl fluoride, B) complex trisiloxane compound.

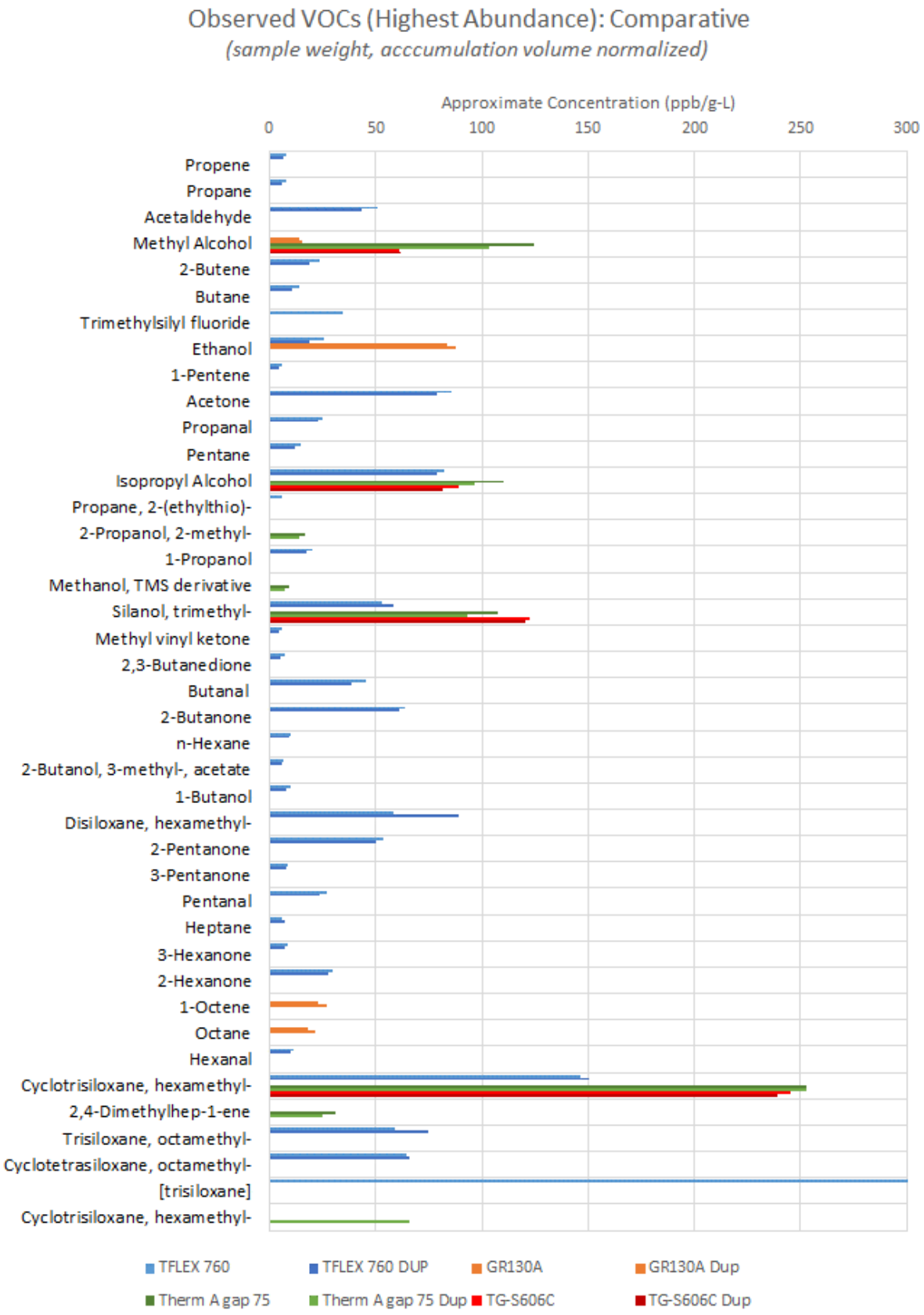

Figure 2. Highest abundance outgassing compounds (and approximate concentrations) of 4 thermal filler materials held at 80 C for ~48 hours under N_2. Reported concentrations normalized to sample weight and accumulation volume (g-L basis), providing a convenient way to quickly evaluate which compounds originated from which samples, and to what extent.

Detection of a sulfur-containing compound in Therm-a-Gap material

An unusual sulfur-containing compound- *2-methyl-2-undecanethiol*- was detected in trace concentrations the Therm-a-Gap 75 material. This corroborates a similar result from an outgassing analysis previously performed on a related material, Therm-a-Gap Gel 30 (see Appendix C). This compound consists of a long alkane chain with a thiol termination (see Figure 3) and, according to at least one source,* is likely present as an additive used to inhibit corrosion.[8] While it may at first appear contradictory that a sulfurous compound would be intentionally used as a corrosion inhibitor, it makes sense when one considers the structure of the molecule. It is likely that the thiol end of this molecule readily binds with any active reaction site on a corrosion-prone material. Once bound, the alkane tail of the molecule would, in combination with adjacent similarly-bound molecules, form a non-reactive, hydrophobic buffer over the surface of the material, thus preventing further reaction/attack from other potentially reactive/corrosive gas-phase species in the system.

A direct comparison between the outgassing profiles of Therm-a-Gap 30 and 75 was performed. Of particular interest in these outgassing screenings was the detection of the *2-methyl-2-undecanethiol* in both of the Therm-a-Gap materials, as it has been the general approach to flag any sulfur-containing compound in the outgassing profile of a material as being "of potential concern." This is shown in Figure 3, in which the normalized concentrations of the compound are presented. The Gel 30 formulation underwent 2 accumulation conditions- room temperature and 80 ºC; both are presented here. The detected levels of the thio-alkane compound were nominally similar for both temperature conditions in the Gel 30. The detected levels were slightly higher in the Gel 75.

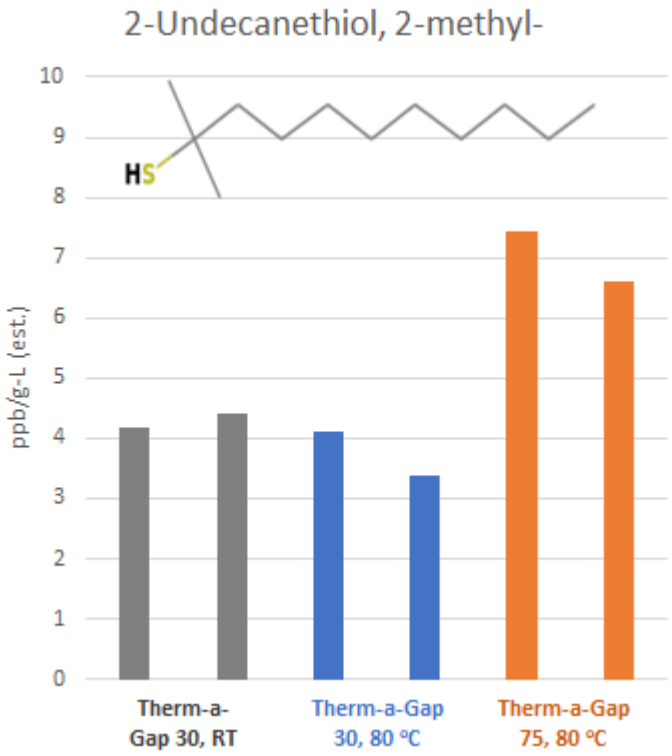

Figure 3. Estimated concentrations of the 2-methyl-2-undecanethiol in Therm-a-Gap outgassing study (normalized for sample weight, accumulation volume).

*pointed out to me by Yibin Zhang, which she uncovered in her literature search

A direct comparison between the Gel 30 and Gel 75 formulations was also performed for the highest abundance compounds observed in the respective analyses. This is shown below in Figure 4. In this plot, the differences in the estimated compound concentrations between the respective materials can be easily seen (e.g., the Gel 30 formulation outgasses higher amounts of siloxanes and silanol than the Gel 75).

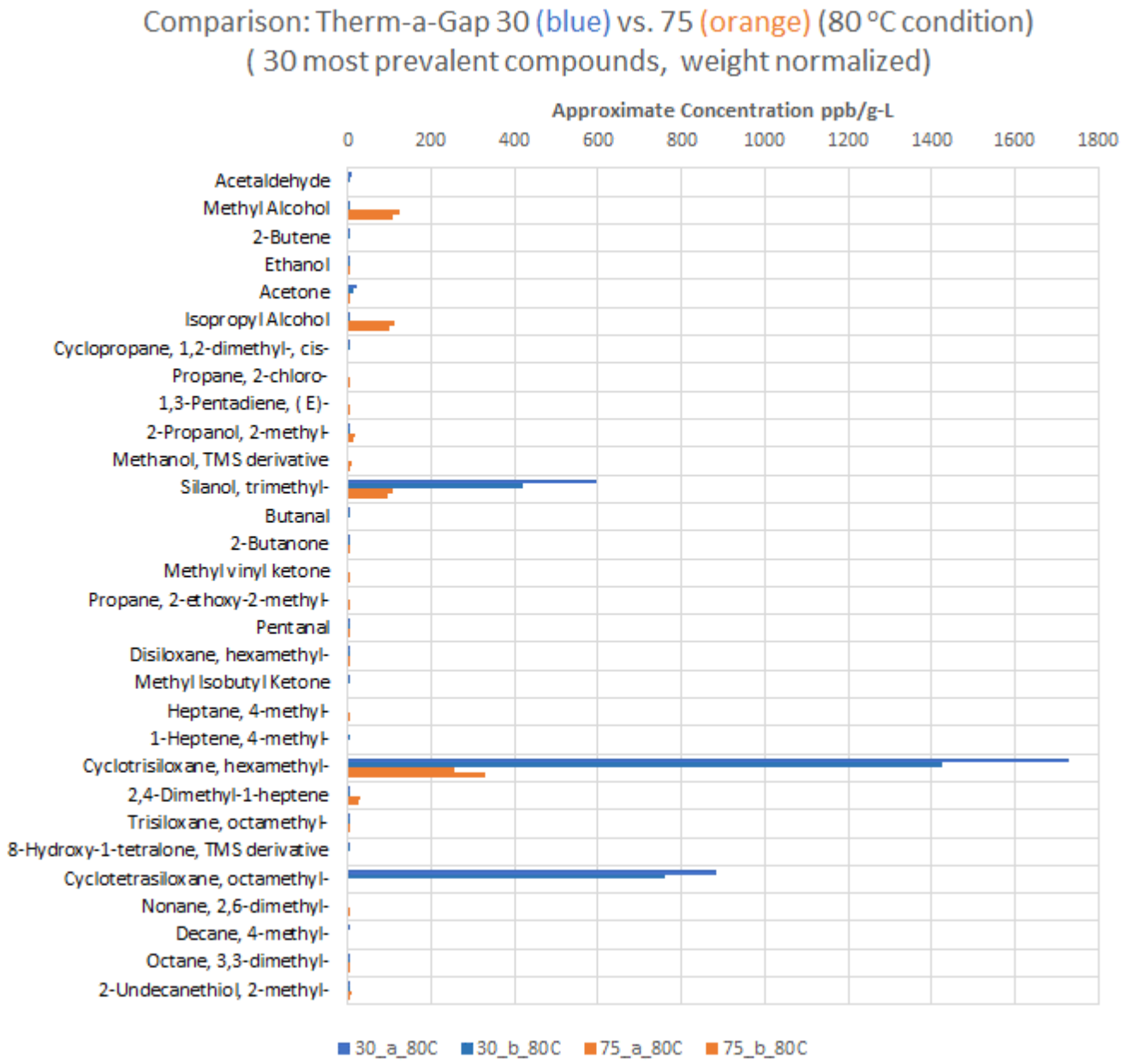

Figure 4. *Highest abundance outgassing compounds (and approximate concentrations) of Therm-a-gap Gel 30 and Gel 75 materials held at 80 C under N_2 for 1 week and 48 hours, respectively. Reported concentrations normalized to sample weight and accumulation volume (g-L basis), providing a convenient way to quickly evaluate which compounds originated from which samples, and to what extent.*

Discussion

Many materials tend to exhibit outgassing characteristics far more complex than a mere evaluation of the stated nominal composition would suggest. It is inevitable that impurities, residual unreacted compounds from the original synthesis of the material, additives, or peripheral compounds used in various processing steps will be present in the bulk material and likely contribute to its overall outgassing profile. This appears to be the materials interrogated in this study. In the headspace analysis used to characterize the gas-phase compounds evolved from the base materials, a complex "soup" of organic compounds was observed, most of which are not obviously representative of the stated chemical composition of the materials themselves.

The general approach to interpreting a material screening of this type is to evaluate the inventory of observed compounds for certain classes known to be reactive or present the potential for active chemistry to take place in a system. In general, there are categories of compound deemed to be of particular interest in the materials community including acids, halogenated compounds, and sulfur containing compounds (though it should be noted that interest from a reactivity standpoint is not always relegated to those categories alone. Conversely, the detection of a potentially corrosive compound in the outgassing profile of a material does not necessarily imply a risk associated with its use. Factors such as system geometry, the amount of material used, and the types of materials present in the system all affect the potential to realize a reactive environment). Several compounds falling into these general categories were observed in the outgassing screening of the 4 materials in this study, summarized in Table I of this report.

It is impossible to predict from an analysis of this type alone the potential for active chemistries to manifest in whatever system or application the material will eventually be used. However, this and similar analyses are intended to provide the basis from which materials SMEs and chemists who are more familiar with the system can evaluate any risks posed by the use of the material in a more informed manner.

References

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3. Brown, J. and R. Fuentes, *Addendum to Cryo-GCMS Outgassing Study: Polyphenylene Sulfide (PPS)*. SNL Memo, 2019. **To: Robert Bernstein** (August 15): p. 1-2.

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6. Brown, J. and R. Fuentes, *Study of Poly(etherketoneketone) (PEKK): Outgassing Characteristics and Likely Residual Synthesis Impurities.* SAND report, 2020. **SAND2020-7393R**, p. 1-10

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8. Verma, C. et al., *Thiol (-SH) substituent as functional motif for effective corrosion protection: A review on current advancements and future directions.* J. Molecular Liquids Volume 324, 15 February 2021, 115111

Appendix A. Total observed compounds (in order of highest concentration, log scale)

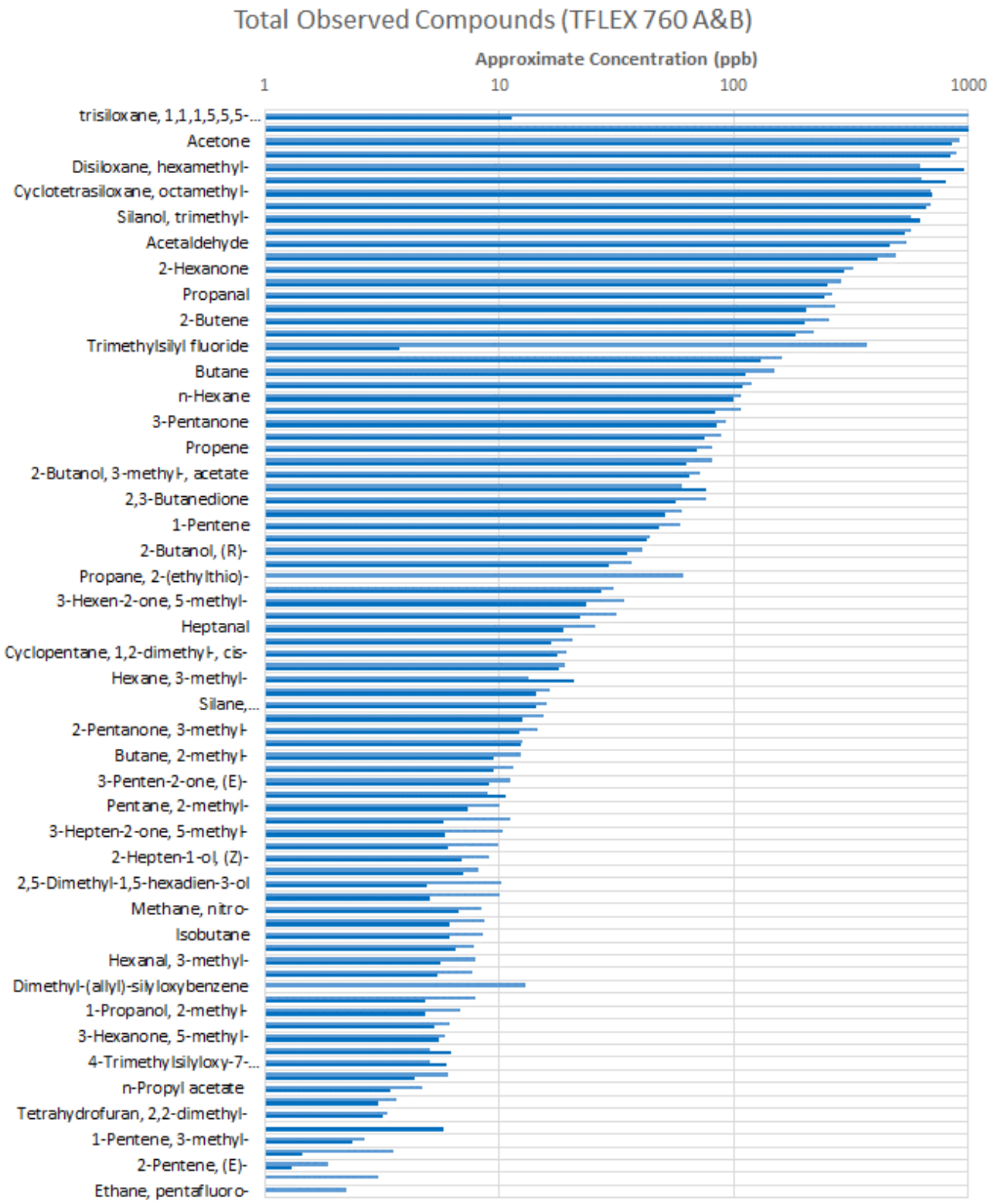

Figure A1. Total observed compounds and estimated concentrations in headspace of TFLEX 760 samples (presented on log plot). (Samples held under N_2 for ~ 48 hours at 80 °C; cooled to room temperature before undergoing headspace analysis via cryofocusing GC/MS.

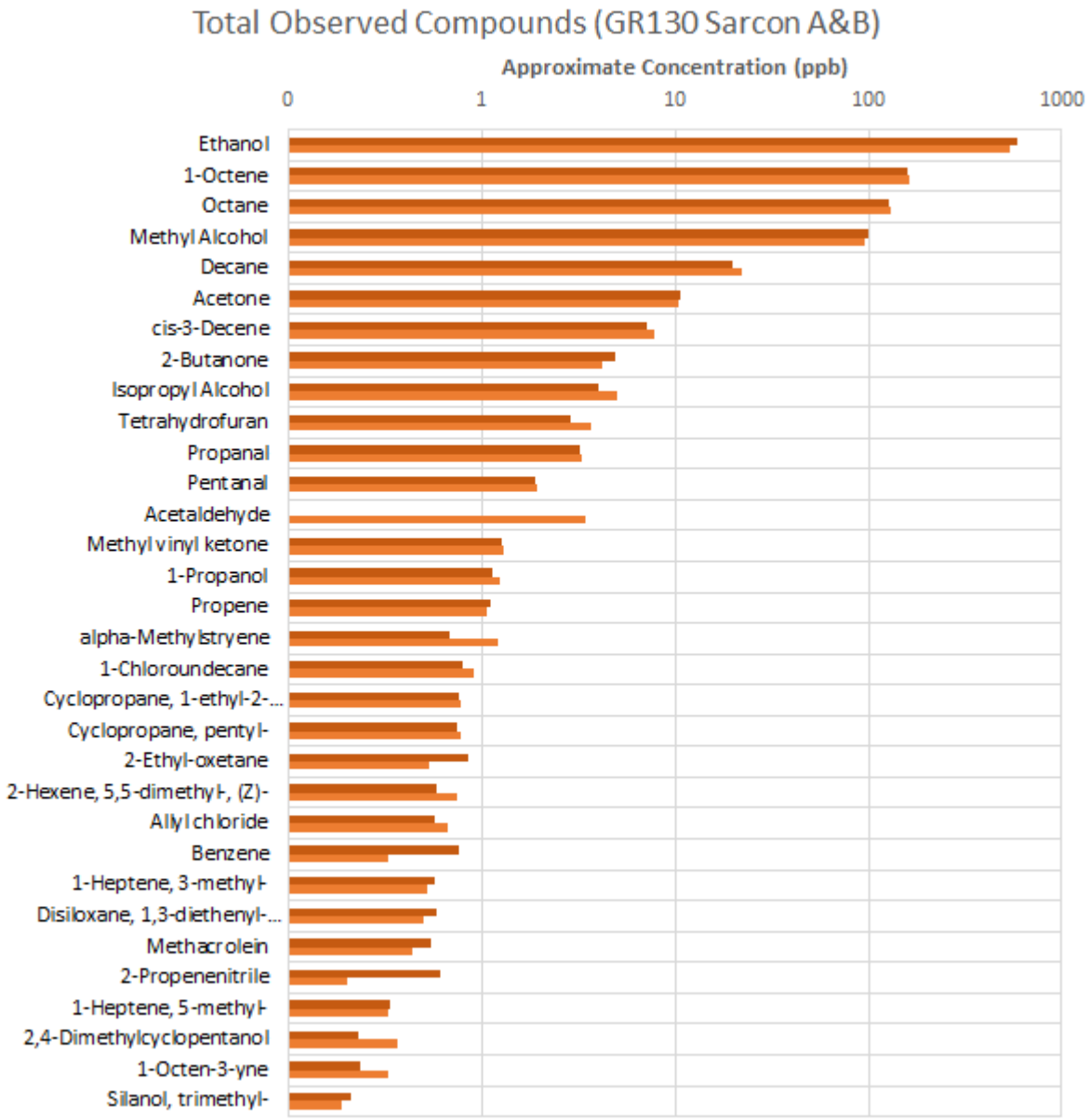

Figure A2. Total observed compounds and estimated concentrations in headspace of GR130 Sarcon samples (presented on log plot). (Samples held under N_2 for ~48 hours at 80 °C; cooled to room temperature before undergoing headspace analysis via cryofocusing GC/MS.

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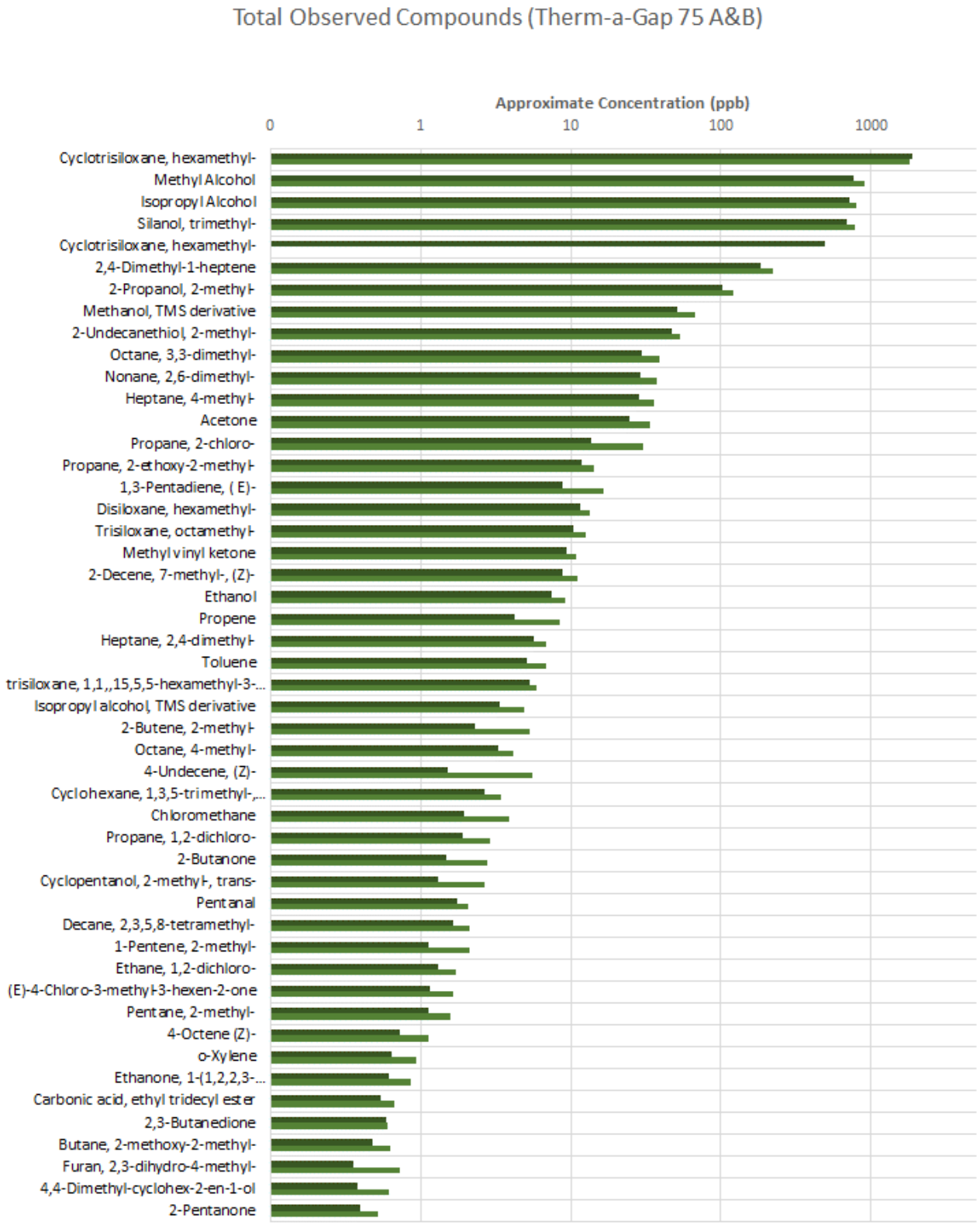


Figure A3. Total observed compounds and estimated concentrations in headspace of Therm-a-Gap 75 samples (presented on log plot). (Samples held under N_2 for ~48 hours at 80 °C; cooled to room temperature before undergoing headspace analysis via cryofocusing GC/MS.

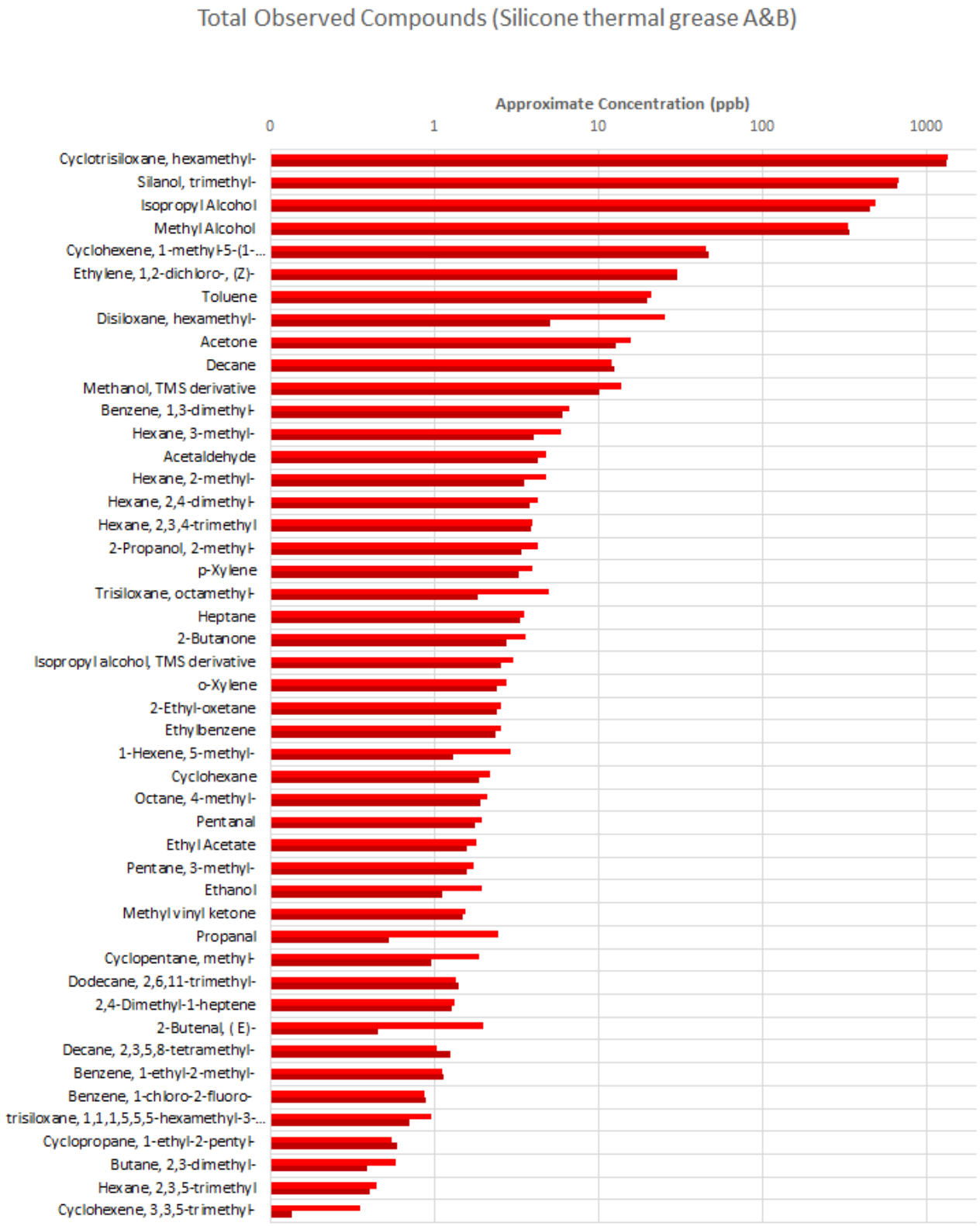


Figure A4. Total observed compounds and estimated concentrations in headspace of silicone grease samples (presented on log plot). (Samples held under N_2 for ~48 hours at 80 °C; cooled to room temperature before undergoing headspace analysis via cryofocusing GC/MS.

Appendix B. TICs and Peak Identifications from Headspace Analyses (cryo-GC/MS)

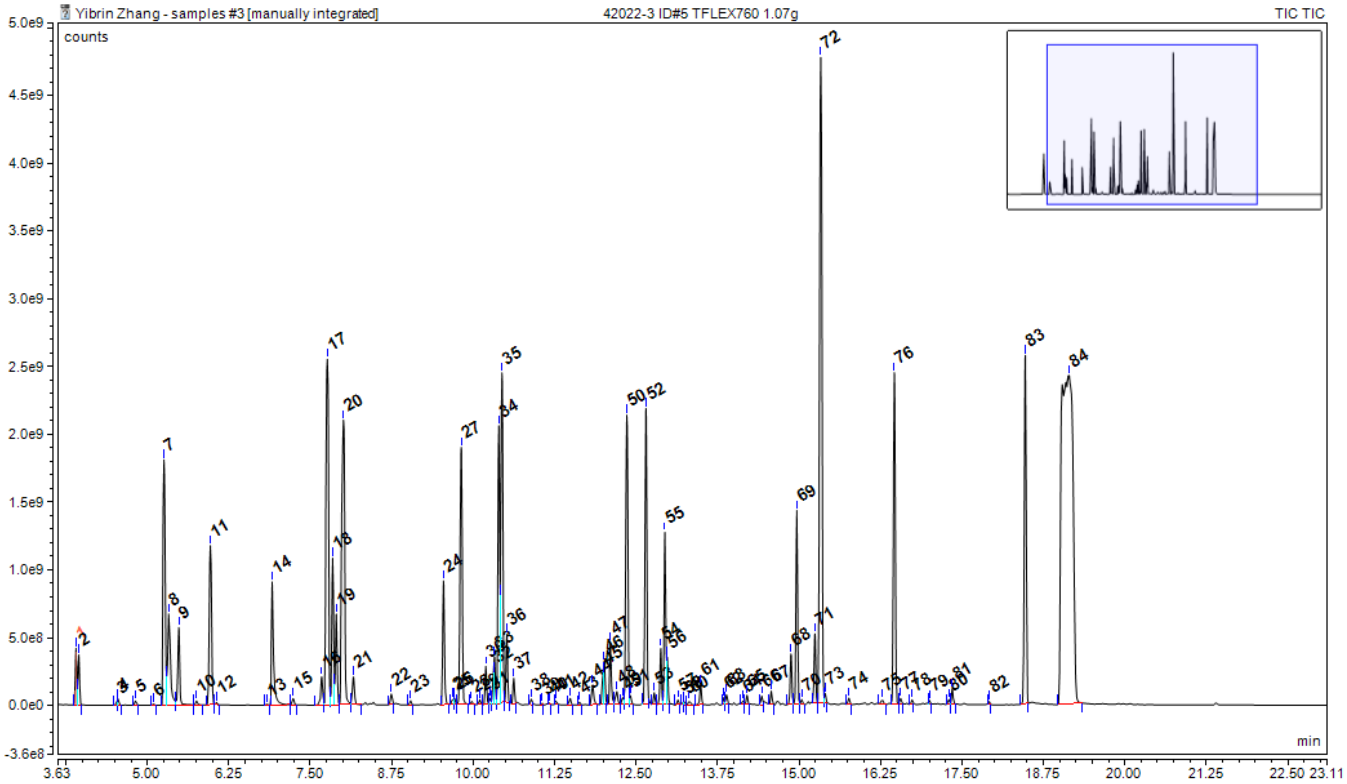


Figure B1. TIC for TFLEX 760-A: cryo-GC/MS headspace analysis. Peak indices correspond to compounds listed below in Table B1.

Table B1. Observed outgassing compounds from TFLEX 760 A: cryo-GC/MS headspace analysis. Peak indices correspond to peaks labeled in the chromatogram presented in Figure B1.

Peak #	ID	RT	CAS#	Formula	Match	Area	Approx Conc. (ppb)
1	Propene	3.904	115-07-1	C3H6	973	10522374	80.7
2	Propane	3.949	74-98-6	C3H8	858	10535930	80.8
3	Silane, difluorodimethyl-	4.52	353-66-2	C2H6F2Si	904	398495	3.1
4	Cyclopropane	4.551	75-19-4	C3H6	842	1453332	11.2
5	Isobutane	4.819	75-28-5	C4H10	922	1112569	8.5
6	Ethane, pentafluoro-	5.095	354-33-6	C2HF5	811	291340	2.2
7	Acetaldehyde	5.255	75-07-0	C2H4O	926	71169260	546.1
8	2-Butene	5.326	107-01-7	C4H8	756	33035778	253.5
9	Butane	5.483	106-97-8	C4H10	943	19340062	148.4
10	2-Butene, (Z)-	5.751	590-18-1	C4H8	887	1031958	7.9
11	Trimethylsilyl fluoride	5.965	420-56-4	C3H9FSi	936	48180105	369.7
12	2-Butene, (E)-	6.064	624-64-6	C4H8	958	470435	3.6
13	2-Pentene, (E)-	6.836	646-04-8	C5H10	901	241716	1.9
14	Ethanol	6.914	64-17-5	C2H6O	901	35286691	270.8
15	Butane, 2-methyl-	7.237	78-78-4	C5H12	876	1619080	12.4
16	1-Pentene	7.676	109-67-1	C5H10	940	7667442	58.8
17	Acetone	7.761	67-64-1	C3H6O	857	119374601	916.0
18	Propanal	7.843	123-38-6	C3H6O	916	34330010	263.4
19	Pentane	7.901	109-66-0	C5H12	907	20833916	159.9
20	Isopropyl Alcohol	8.01	67-63-0	C3H8O	920	115109212	883.3
21	Propane, 2-(ethylthio)-	8.163	5145-99-3	C5H12S	624	7936193	60.9
22	2-Propanol, 2-methyl-	8.744	75-65-0	C4H10O	859	2461635	18.9
23	Isobutylene epoxide	9.037	558-30-5	C4H8O	866	1006100	7.7
24	1-Propanol	9.543	71-23-8	C3H8O	865	28525655	218.9
25	Methane, nitro-	9.683	75-52-5	CH3NO2	714	1083330	8.3
26	Pentane, 2-methyl-	9.713	107-83-5	C6H14	804	1302762	10.0
27	Silanol, trimethyl-	9.816	1066-40-6	C3H10OSi	910	73987739	567.7
28	Furan, 2,3-dihydro-	9.972	1191-99-7	C4H6O	777	787641	6.0
29	Pentane, 3-methyl-	10.101	96-14-0	C6H14	898	1163023	8.9
30	Methyl vinyl ketone	10.193	78-94-4	C4H6O	938	7744334	59.4
31	1-Pentene, 2-methyl-	10.261	763-29-1	C6H12	917	1492099	11.4
32	1-Hexene	10.31	592-41-6	C6H12	872	4099827	31.5
33	2,3-Butanedione	10.326	431-03-8	C4H6O2	890	9848433	75.6
34	Butanal	10.39	123-72-8	C4H8O	915	63512677	487.3
35	2-Butanone	10.441	78-93-3	C4H8O	845	89249248	684.8
36	n-Hexane	10.516	110-54-3	C6H14	931	14050214	107.8
37	2-Butanol, (R)-	10.622	14898-79-4	C4H10O	882	5319049	40.8
38	Pentane, 1-propoxy-	10.89	18641-82-2	C8H18O	749	1298690	10.0
39	1-Pentene, 3-methyl-	11.057	760-20-3	C6H12	867	344074	2.6
40	2-Pentenal, (E)-	11.166	1576-87-0	C5H8O	869	459368	3.5
41	1-Propanol, 2-methyl-	11.271	78-83-1	C4H10O	815	886978	6.8
42	Dimethyl-(allyl)-silyloxybenzene	11.485	66998-68-3	C11H16OSi	742	1685665	12.9
43	Amylene hydrate	11.632	75-85-4	C5H12O	838	656993	5.0
44	3-Pentenal, 4-methyl-	11.832	5362-50-5	C6H10O	839	5673836	43.5
45	Butanal, 3-methyl-	11.98	590-86-3	C5H10O	877	4769581	36.6
46	2-Butanol, 3-methyl-, acetate	12.009	5343-96-4	C7H14O2	703	9353805	71.8
47	1-Butanol	12.104	71-36-3	C4H10O	874	14022208	107.6
48	Butanal, 2-methyl-	12.203	96-17-3	C5H10O	847	3981778	30.6
49	Acetate, 4-hydroxy-3-methyl-2-butenyl-	12.295		C7H12O3	815	1636391	12.6
50	Disiloxane, hexamethyl-	12.356	107-46-0	C6H18OSi2	926	81425496	624.8
51	Hexane, 3-methyl-	12.414	589-34-4	C7H16	893	1741459	13.4
52	2-Pentanone	12.652	107-87-9	C5H10O	927	74519483	571.8
53	Cyclopentane, 1,2-dimethyl-, cis-	12.778	1192-18-3	C7H14	920	2499123	19.2
54	3-Pentanone	12.88	96-22-0	C5H10O	912	12077808	92.7
55	Pentanal	12.941	110-62-3	C5H10O	881	37473759	287.5
56	Heptane	12.975	142-82-5	C7H16	946	7781482	59.7
57	Furan, 2,5-dihydro-2,5-dimethyl-	13.142	59242-27-2	C6H10O	823	1128434	8.7
58	Tetrahydrofuran, 2,2-dimethyl-	13.22	1003-17-4	C6H12O	806	432228	3.3
59	n-Propyl acetate	13.25	109-60-4	C5H10O2	814	610081	4.7
60	2-Hepten-1-ol, (Z)-	13.32	55454-22-3	C7H14O	729	1170659	9.0
61	3-Hexen-2-one, 5-methyl-	13.492	5166-53-0	C7H12O	843	4445924	34.1
62	3-Penten-2-one, (E)-	13.846	3102-33-8	C5H8O	888	1437384	11.0
63	Methyl Isobutyl Ketone	13.887	108-10-1	C6H12O	874	2019389	15.5
64	3-Pentanone, 2-methyl-	14.135	565-69-5	C6H12O	835	800182	6.1
65	2-Pentanone, 3-methyl-	14.2	565-61-7	C6H12O	894	1889021	14.5
66	1,5-Dimethyl-6-oxa-bicyclo[3.1.0]hexane	14.427	82461-31-2	C7H12O	768	2131150	16.4
67	Pentanal, 3-methyl-	14.574	15877-57-3	C6H12O	877	2660141	20.4
68	3-Hexanone	14.876	589-38-8	C6H12O	900	11539382	88.5
69	2-Hexanone	14.965	591-78-6	C6H12O	948	41839533	321.0
70	2-Octene	15.043	111-67-1	C8H16	842	1282423	9.8
71	Hexanal	15.244	66-25-1	C6H12O	824	15405746	118.2
72	Cyclotrisiloxane, hexamethyl-	15.332	541-05-9	C6H18O3Si3	898	203806440	1563.9
73	Silane, diisopropylmethylisopropoxy-	15.4		C10H24OSi	677	2076102	15.9
74	3-Hepten-2-one, 5-methyl-	15.764	5090-16-4	C8H14O	782	1337725	10.3
75	2,5-Dimethyl-1,5-hexadien-3-ol	16.274	17123-63-6	C8H14O	729	1322603	10.1
76	Trisiloxane, octamethyl-	16.461	107-51-7	C8H24O2Si3	912	82218682	630.9
77	Hexanal, 3-methyl-	16.56	19269-28-4	C7H14O	778	1022187	7.8
78	4-Heptanone	16.733	123-19-3	C7H14O	837	1061267	8.1
79	3-Hexanone, 5-methyl-	17.002	623-56-3	C7H14O	808	758869	5.8
80	Nonane	17.298	111-84-2	C9H20	866	1003953	7.7
81	Heptanal	17.352	111-71-7	C7H14O	897	3320140	25.5
82	4-Trimethylsilyloxy-7-methylcoumarin	17.92		C13H16O3Si	644	656009	5.0
83	Cyclotetrasiloxane, octamethyl-	18.471	556-67-2	C8H24O4Si4	901	90075632	691.2
84	trisiloxane, 1,1,1,5,5,5-hexamethyl-3-[(tr	19.145		C9H28O3Si4	928	491243680	3769.4
	Other					33832477	259.6
					Total =	2110389685	16193.5
				Response Factor =		26116766	200.4

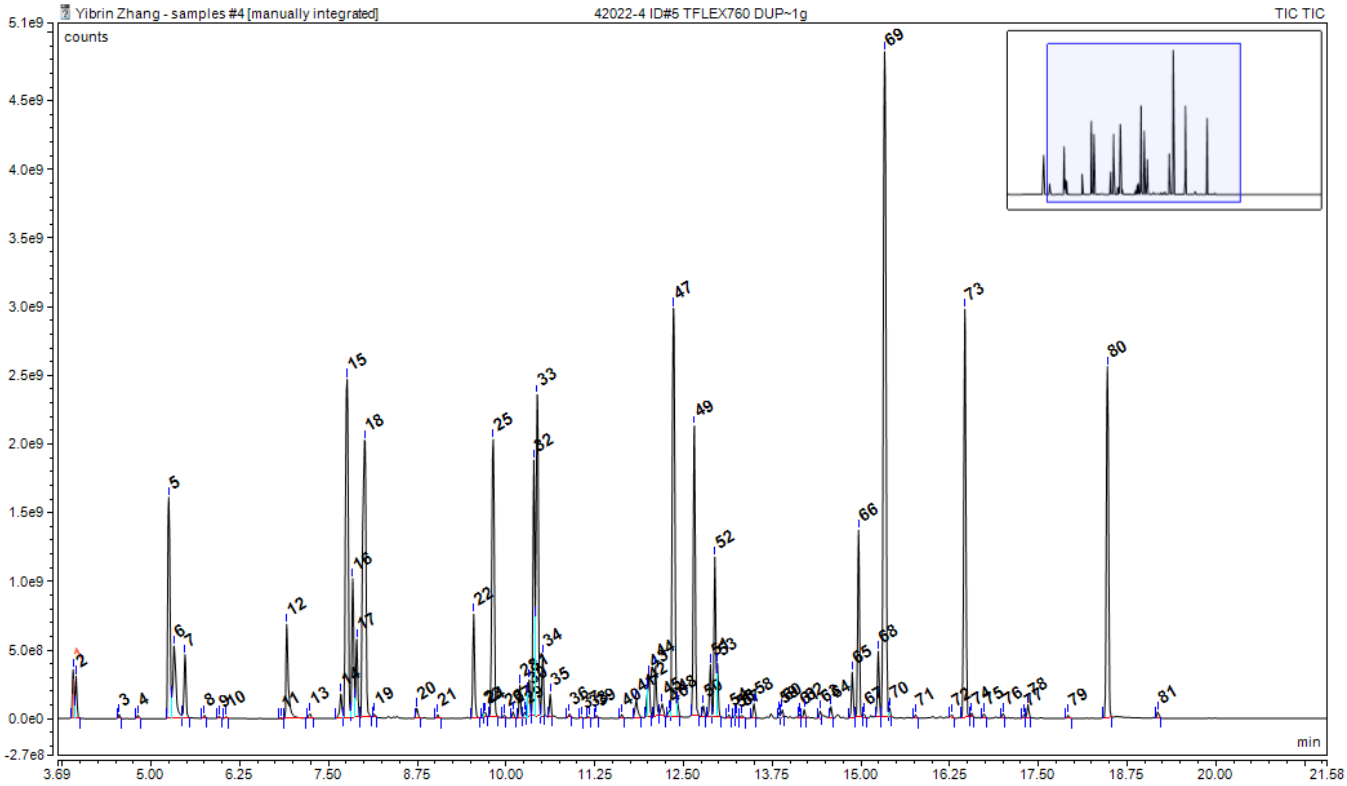


Figure B2. TIC for TFLEX 760 B: cryo-GC/MS headspace analysis. Peak indices correspond to compounds listed below in Table B2.

Table B2. Observed outgassing compounds from TFLEX 760 B: cryo-GC/MS headspace analysis. Peak indices correspond to peaks labeled in the chromatogram presented in Figure B2.

Peak #	ID	RT	CAS#	Formula	Match	Area	Approx Conc. (ppb)
1	Propene	3.901	115-07-1	C3H6	954	9094787	69.8
2	Propane	3.942	74-98-6	C3H8	944	8178099	62.8
3	Cyclopropane	4.547	75-19-4	C3H6	961	752570	5.8
4	Isobutane	4.813	75-28-5	C4H10	879	801806	6.2
5	Acetaldehyde	5.248	75-07-0	C2H4O	934	59997708	460.4
6	2-Butene	5.323	107-01-7	C4H8	797	26066683	200.0
7	Butane	5.476	106-97-8	C4H10	938	14626960	112.2
8	2-Butene, (Z)-	5.748	590-18-1	C4H8	880	632140	4.9
9	Trimethylsilyl fluoride	5.955	420-56-4	C3H9FSi	686	486953	3.7
10	2-Butene, (E)-	6.057	624-64-6	C4H8	928	394404	3.0
11	2-Pentene, (E)-	6.833	646-04-8	C5H10	902	170628	1.3
12	Ethanol	6.908	64-17-5	C2H6O	915	26481495	203.2
13	Butane, 2-methyl-	7.234	78-78-4	C5H12	877	1229942	9.4
14	1-Pentene	7.673	109-67-1	C5H10	942	6252238	48.0
15	Acetone	7.761	67-64-1	C3H6O	874	110124413	845.0
16	Propanal	7.84	123-38-6	C3H6O	919	31472513	241.5
17	Pentane	7.897	109-66-0	C5H12	917	16872215	129.5
18	Isopropyl Alcohol	8.006	67-63-0	C3H8O	929	109751408	842.1
19	2-Pentene, (E)-	8.146	646-04-8	C5H10	830	750383	5.8
20	2-Propanol, 2-methyl-	8.741	75-65-0	C4H10O	874	2316174	17.8
21	Isobutylene epoxide	9.033	558-30-5	C4H8O	876	844382	6.5
22	1-Propanol	9.543	71-23-8	C3H8O	831	23892718	183.3
23	Methane, nitro-	9.68	75-52-5	CH3NO2	785	869937	6.7
24	Pentane, 2-methyl-	9.71	107-83-5	C6H14	812	955422	7.3
25	Silanol, trimethyl-	9.819	1066-40-6	C3H10OSi	917	81458022	625.0
26	Furan, 2,3-dihydro-	9.975	1191-99-7	C4H6O	718	562813	4.3
27	Pentane, 3-methyl-	10.098	96-14-0	C6H14	901	1377950	10.6
28	Methyl vinyl ketone	10.193	78-94-4	C4H6O	923	6600459	50.6
29	1-Pentene, 2-methyl-	10.258	763-29-1	C6H12	905	1230291	9.4
30	1-Hexene	10.309	592-41-6	C6H12	908	2882682	22.1
31	2,3-Butanedione	10.326	431-03-8	C4H6O2	876	7311506	56.1
32	Butanal	10.39	123-72-8	C4H8O	916	53548611	410.9
33	2-Butanone	10.438	78-93-3	C4H8O	884	85312553	654.6
34	n-Hexane	10.516	110-54-3	C6H14	931	12985903	99.6
35	2-Butanol, (R)-	10.622	14898-79-4	C4H10O	876	4592121	35.2
36	Pentane, 1-propoxy-	10.89	18641-82-2	C8H18O	737	655171	5.0
37	1-Pentene, 3-methyl-	11.057	760-20-3	C6H12	760	305332	2.3
38	2-Pentenal, (E)-	11.166	1576-87-0	C5H8O	760	187910	1.4
39	1-Propanol, 2-methyl-	11.271	78-83-1	C4H10O	759	632240	4.9
40	Amylene hydrate	11.628	75-85-4	C5H12O	766	803855	6.2
41	3-Pentenal, 4-methyl-	11.832	5362-50-5	C6H10O	801	5566174	42.7
42	Butanal, 3-methyl-	11.996	590-86-3	C5H10O	823	3788630	29.1
43	2-Butanol, 3-methyl-, acetate	12.009	5343-96-4	C7H14O2	708	8459440	64.9
44	1-Butanol	12.104	71-36-3	C4H10O	842	10843670	83.2
45	Butanal, 2-methyl-	12.2	96-17-3	C5H10O	702	3550649	27.2
46	Acetate, 4-hydroxy-3-methyl-2-butenyl-	12.295		C7H12O3	645	1602039	12.3
47	Disiloxane, hexamethyl-	12.356	107-46-0	C6H18OSi2	905	124198825	953.0
48	Hexane, 3-methyl-	12.414	589-34-4	C7H16	800	2692275	20.7
49	2-Pentanone	12.652	107-87-9	C5H10O	919	70147196	538.3
50	Cyclopentane, 1,2-dimethyl-, cis-	12.778	1192-18-3	C7H14	751	2285401	17.5
51	3-Pentanone	12.88	96-22-0	C5H10O	890	10988378	84.3
52	Pentanal	12.941	110-62-3	C5H10O	848	32701902	250.9
53	Heptane	12.979	142-82-5	C7H16	946	9878633	75.8
54	Furan, 2,5-dihydro-2,5-dimethyl-	13.142	59242-27-2	C6H10O	802	796485	6.1
55	Tetrahydrofuran, 2,2-dimethyl-	13.23	1003-17-4	C6H12O	823	413079	3.2
56	n-Propyl acetate	13.237	109-60-4	C5H10O2	794	443153	3.4
57	2-Hepten-1-ol, (Z)-	13.315	55454-22-3	C7H14O	676	898201	6.9
58	3-Hexen-2-one, 5-methyl-	13.492	5166-53-0	C7H12O	833	3052907	23.4
59	3-Penten-2-one, (E)-	13.849	3102-33-8	C5H8O	907	1173882	9.0
60	Methyl Isobutyl Ketone	13.89	108-10-1	C6H12O	841	1635311	12.5
61	3-Pentanone, 2-methyl-	14.135	565-69-5	C6H12O	846	686750	5.3
62	2-Pentanone, 3-methyl-	14.203	565-61-7	C6H12O	888	1583985	12.2
63	1,5-Dimethyl-6-oxa-bicyclo[3.1.0]hexane	14.427	82461-31-2	C7H12O	777	1878073	14.4
64	Pentanal, 3-methyl-	14.577	15877-57-3	C6H12O	862	2178987	16.7
65	3-Hexanone	14.876	589-38-8	C6H12O	907	9702426	74.4
66	2-Hexanone	14.965	591-78-6	C6H12O	937	38355112	294.3
67	2-Octene	15.043	111-67-1	C8H16	851	788444	6.0
68	Hexanal	15.244	66-25-1	C6H12O	880	14166487	108.7
69	Cyclotrisiloxane, hexamethyl-	15.332	541-05-9	C6H18O3Si3	902	209699212	1609.1
70	Silane, diisopropylmethylisopropoxy-	15.4		C10H24OSi	638	1853863	14.2
71	3-Hepten-2-one, 5-methyl-	15.764	5090-16-4	C8H14O	783	757819	5.8
72	2,5-Dimethyl-1,5-hexadien-3-ol	16.274	17123-63-6	C8H14O	758	634995	4.9
73	Trisiloxane, octamethyl-	16.461	107-51-7	C8H24O2Si3	906	104181725	799.4
74	Hexanal, 3-methyl-	16.56	19269-28-4	C7H14O	761	726455	5.6
75	4-Heptanone	16.733	123-19-3	C7H14O	811	914408	7.0
76	3-Hexanone, 5-methyl-	17.002	623-56-3	C7H14O	824	719297	5.5
77	Nonane	17.298	111-84-2	C9H20	825	706987	5.4
78	Heptanal	17.352	111-71-7	C7H14O	879	2438461	18.7
79	4-Trimethylsilyloxy-7-methylcoumarin	17.92		C13H16O3Si	622	777666	6.0
80	Cyclotetrasiloxane, octamethyl-	18.471	556-67-2	C8H24O4Si4	900	91680279	703.5
81	2,2,7,7-Tetramethyloctane	19.182	1071-31-4	C12H26	837	1472213	11.3
	Other					48714570	373.8
					Total =	1543197838	11841.3
				Response Factor =		26116766	200.4

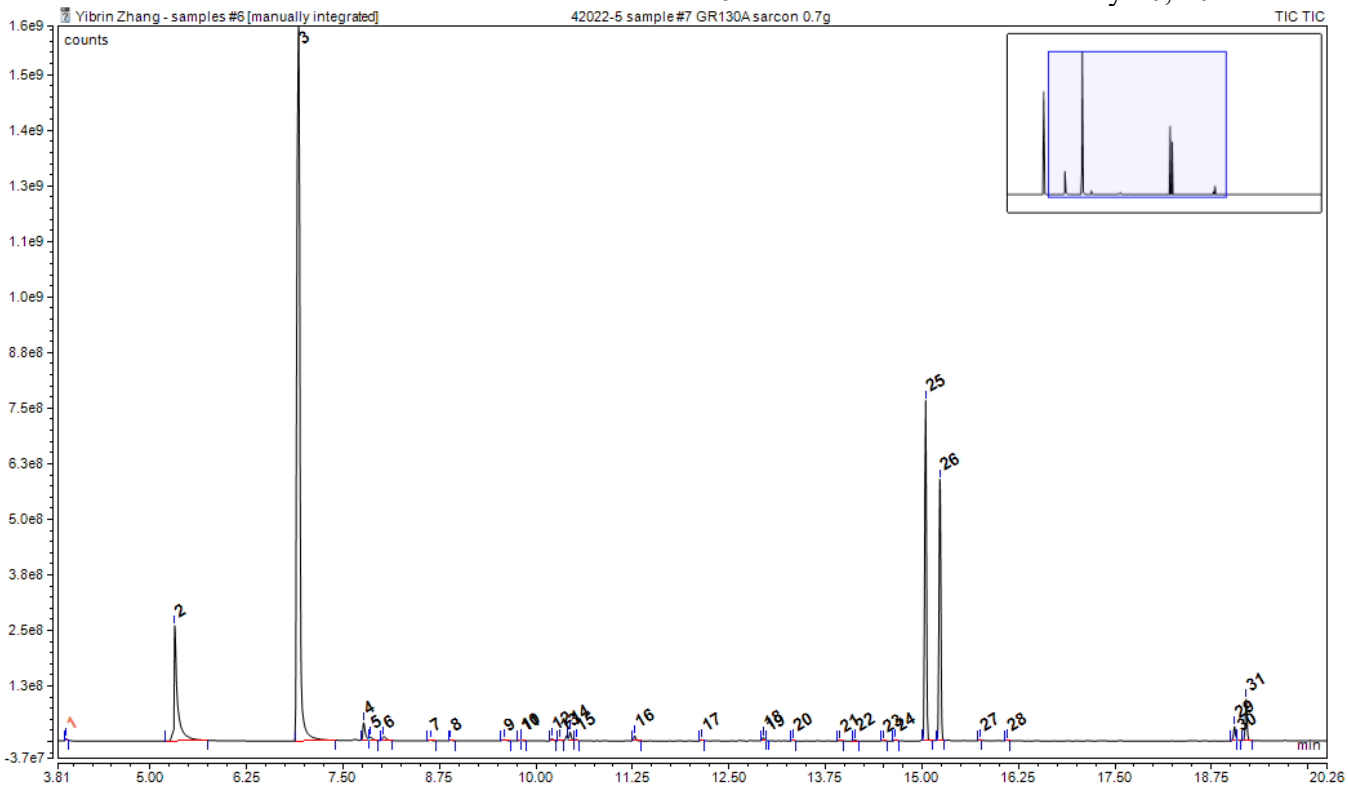


Figure B3. TIC for GR130 Sarcon-A: cryo-GC/MS headspace analysis. Peak indices correspond to compounds listed below in Table B3.

Table B3. Observed outgassing compounds from GR130 Sarcon-A: cryo-GC/MS headspace analysis. Peak indices correspond to peaks labeled in the chromatogram presented in Figure B3.

Peak #	ID	RT	CAS#	Formula	Match	Area	Approx Conc. (ppb)
1	Propene	3.915	115-07-1	C3H6	886	143775	1.10
2	Methyl Alcohol	5.316	67-56-1	CH4O	975	12916190	99.11
3	Ethanol	6.921	64-17-5	C2H6O	910	75953930	582.81
4	Acetone	7.765	67-64-1	C3H6O	862	1400098	10.74
5	Propanal	7.853	123-38-6	C3H6O	837	418418	3.21
6	Isopropyl Alcohol	8.023	67-63-0	C3H8O	887	522195	4.01
7	2-Propenenitrile	8.629	107-13-1	C3H3N	893	78881	0.61
8	Allyl chloride	8.894	107-05-1	C3H5Cl	909	75034	0.58
9	1-Propanol	9.584	71-23-8	C3H8O	830	149193	1.14
10	Methacrolein	9.799	78-85-3	C4H6O	813	71043	0.55
11	Silanol, trimethyl-	9.82	1066-40-6	C3H10OSi	782	27454	0.21
12	Methyl vinyl ketone	10.203	78-94-4	C4H6O	915	164919	1.27
13	Cyclopropane, 1-ethyl-2-methyl-,cis-	10.305	19781-68-1	C6H12	804	100099	0.77
14	2-Butanone	10.438	78-93-3	C4H8O	907	631112	4.84
15	2-Ethyl-oxetane	10.516		C5H10O	867	109686	0.84
16	Tetrahydrofuran	11.278	109-99-9	C4H8O	835	376952	2.89
17	Benzene	12.15	71-43-2	C6H6	925	99560	0.76
18	Pentanal	12.945	110-62-3	C5H10O	823	243902	1.87
19	2,4-Dimethylcyclopentanol	12.972	89794-28-5	C7H14O	771	30250	0.23
20	2-Hexene, 5,5-dimethyl-, (Z)-	13.329	39761-61-0	C8H16	859	76560	0.59
21	1-Octen-3-yne	13.938	17679-92-4	C8H12	804	30612	0.23
22	1-Heptene, 3-methyl-	14.135	4810-09-7	C8H16	788	73620	0.56
23	1-Heptene, 5-methyl-	14.492	13151-04-7	C8H16	780	43509	0.33
24	1-Chloroundecane	14.659	2473-03-2	C11H23Cl	659	102980	0.79
25	1-Octene	15.047	111-66-0	C8H16	911	20837228	159.89
26	Octane	15.23	111-65-9	C8H18	922	16440920	126.15
27	Cyclopropane, pentyl-	15.751	2511-91-3	C8H16	805	97859	0.75
28	Disiloxane, 1,3-diethenyl-1,1,3,3-tetramethyl-	16.101	2627-95-4	C8H18OSi2	819	75396	0.58
29	cis-3-Decene	19.05	19398-86-8	C10H20	840	923001	7.08
30	alpha-Methylstryene	19.09	98-83-9	C9H10	638	87765	0.67
31	Decane	19.199	124-18-5	C10H22	925	2575650	19.76
	Other					3591410	27.56
					Total =	138469202	1062.51
				Response Factor =		26116765.58	200.40

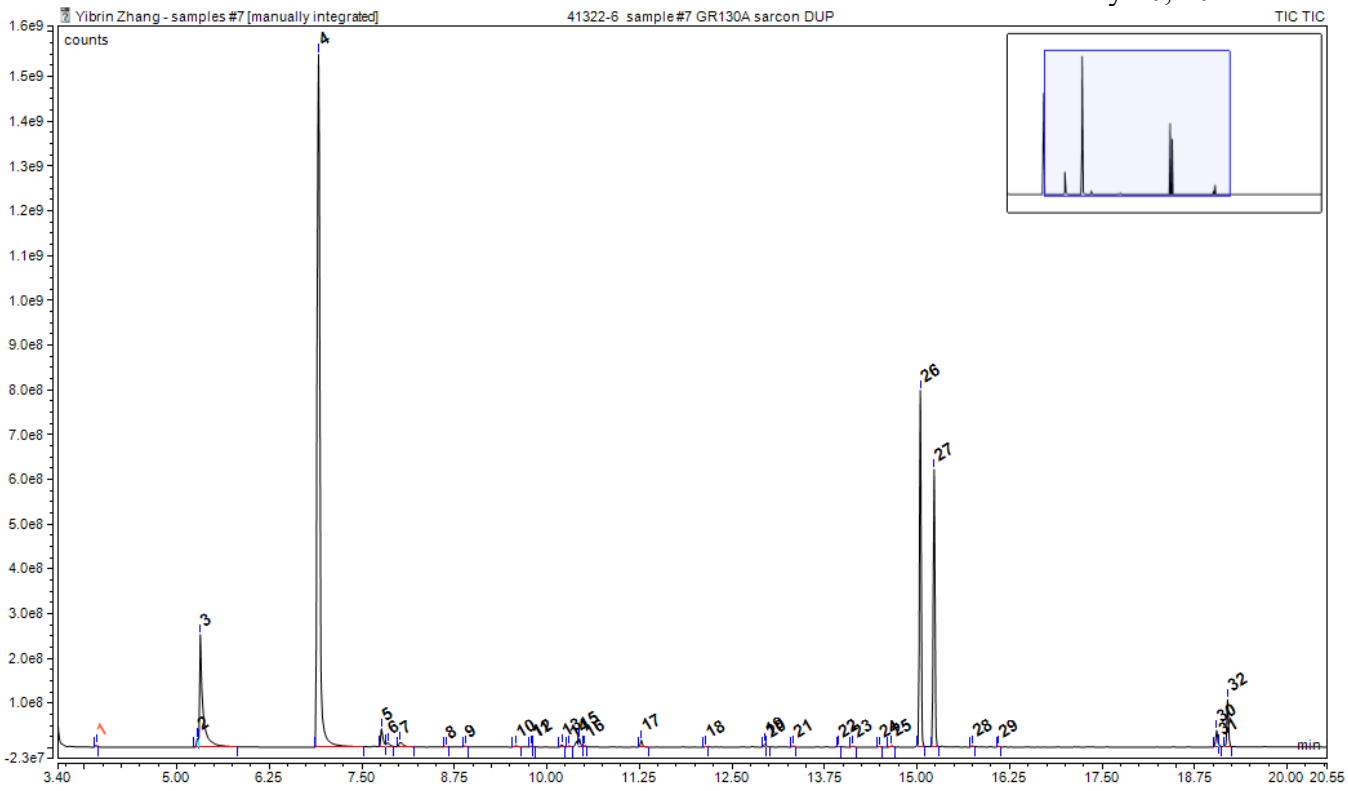


Figure B4. TIC for GR130 Sarcon-B: cryo-GC/MS headspace analysis. Peak indices correspond to compounds listed below in Table B4.

Table B4. Observed outgassing compounds from GR130 Sarcon B: cryo-GC/MS headspace analysis. Peak indices correspond to peaks labeled in the chromatogram presented in Figure B4.

Peak #	ID	RT	CAS#	Formula	Match	Area	Approx Conc. (ppb)
1	Propene	3.915	115-07-1	C3H6	945	138035	1.1
2	Acetaldehyde	5.282	75-07-0	C2H4O	923	449592	3.4
3	Methyl Alcohol	5.316	67-56-1	CH4O	827	12395208	95.1
4	Ethanol	6.915	64-17-5	C2H6O	916	69485121	533.2
5	Acetone	7.765	67-64-1	C3H6O	836	1343216	10.3
6	Propanal	7.85	123-38-6	C3H6O	740	425101	3.3
7	Isopropyl Alcohol	8.02	67-63-0	C3H8O	762	656780	5.0
8	2-Propenenitrile	8.632	107-13-1	C3H3N	750	26320	0.2
9	Allyl chloride	8.894	107-05-1	C3H5Cl	895	85877	0.7
10	1-Propanol	9.581	71-23-8	C3H8O	816	159802	1.2
11	Methacrolein	9.795	78-85-3	C4H6O	848	56430	0.4
	Silanol, trimethyl-	9.81	1066-40-6	C3H10OSi	674	24289	0.2
12	Methyl vinyl ketone	10.2	78-94-4	C4H6O	908	167861	1.3
13	Cyclopropane, 1-ethyl-2-methyl-,cis-	10.302	19781-68-1	C6H12	831	100318	0.8
14	2-Butanone	10.435	78-93-3	C4H8O	919	549374	4.2
15	2-Ethyl-oxetane	10.513		C5H10O	893	68805	0.5
16	Tetrahydrofuran	11.275	109-99-9	C4H8O	843	481232	3.7
17	Benzene	12.142	71-43-2	C6H6	934	42784	0.3
18	Pentanal	12.941	110-62-3	C5H10O	819	250755	1.9
19	2,4-Dimethylcyclopentanol	12.965	89794-28-5	C7H14O	757	48117	0.4
20	2-Hexene, 5,5-dimethyl-, (Z)-	13.329	39761-61-0	C8H16	850	96893	0.7
21	1-Octen-3-yne	13.934	17679-92-4	C8H12	818	42480	0.3
22	1-Heptene, 3-methyl-	14.132	4810-09-7	C8H16	835	68422	0.5
23	1-Heptene, 5-methyl-	14.489	13151-04-7	C8H16	827	42904	0.3
24	1-Chloroundecane	14.659	2473-03-2	C11H23Cl	700	119474	0.9
25	1-Octene	15.043	111-66-0	C8H16	934	21279907	163.3
26	Octane	15.23	111-65-9	C8H18	932	17076595	131.0
27	Cyclopropane, pentyl-	15.751	2511-91-3	C8H16	790	101161	0.8
28	Disiloxane, 1,3-diethenyl-1,1,3,3-tetrar	16.101	2627-95-4	C8H18OSi2	799	65467	0.5
29	cis-3-Decene	19.046	19398-86-8	C10H20	830	1010146	7.8
30	alpha-Methylstryene	19.07	98-83-9	C9H10	763	159233	1.2
31	Decane	19.196	124-18-5	C10H22	920	2887023	22.2
	Other					3051930	23.4
					Total =	132956651	1020.2
				Response Factor =		26116766	200.4

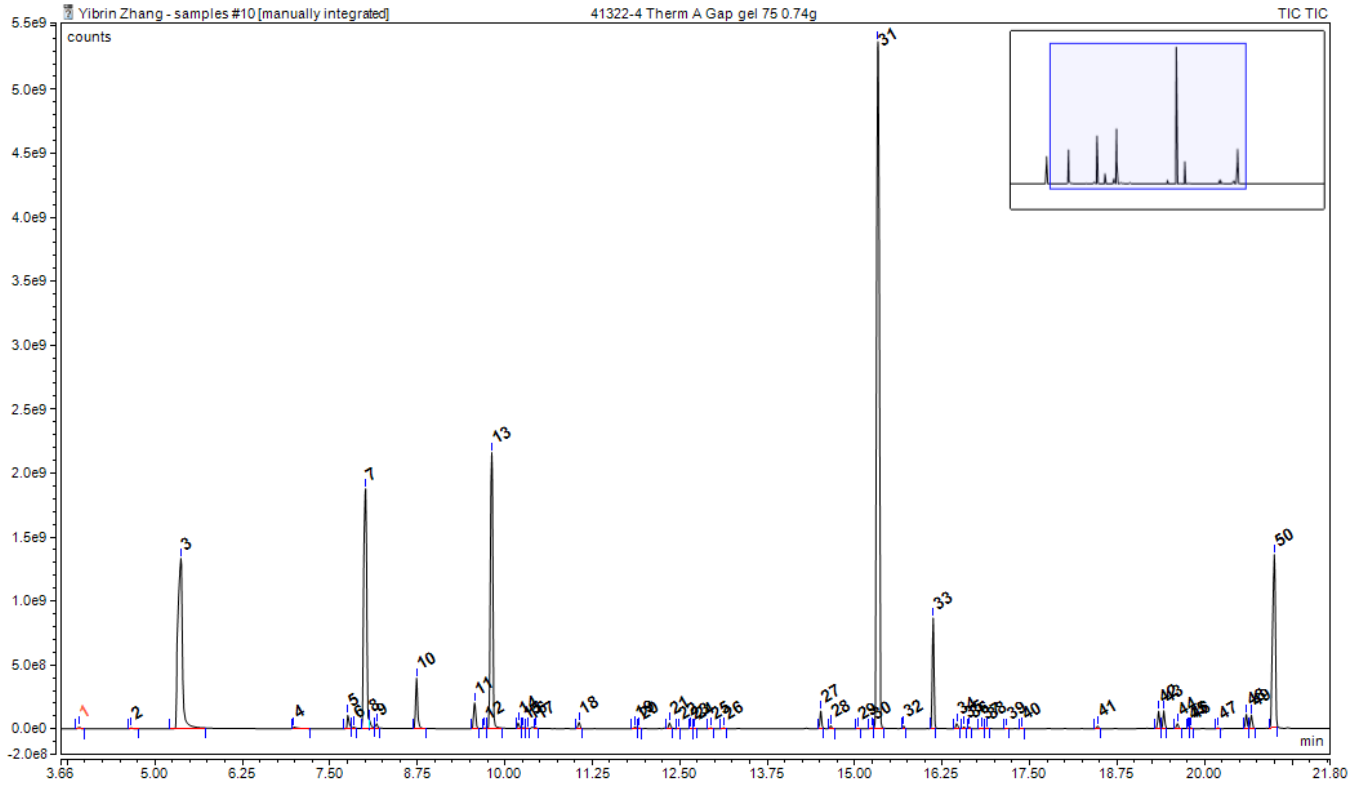


Figure B5. TIC for Therm-a-Gap 75 A: cryo-GC/MS headspace analysis. Peak indices correspond to compounds listed below in Table B5.

Table B5. Observed outgassing compounds from Therma-a-Gap 75 A: cryo-GC/MS headspace analysis. Peak indices correspond to peaks labeled in the chromatogram presented in Figure B5.

Peak #	ID	RT	CAS#	Formula	Match	Area	Approx Conc. (ppb)
1	Propene	3.915	115-07-1	C3H6	983	545259	4.2
2	Chloromethane	4.663	74-87-3	CH3Cl	969	254895	2.0
3	Methyl Alcohol	5.371	67-56-1	CH4O	918	99718111	765.2
4	Ethanol	6.983	64-17-5	C2H6O	925	976473	7.5
5	Acetone	7.755	67-64-1	C3H6O	924	3184362	24.4
6	2-Butene, 2-methyl-	7.843	513-35-9	C5H10	725	302157	2.3
7	Isopropyl Alcohol	8.01	67-63-0	C3H8O	930	93143689	714.7
8	Propane, 2-chloro-	8.057	75-29-6	C3H7Cl	764	1791664	13.7
9	1,3-Pentadiene, (E)-	8.166	2004-70-8	C5H8	888	1151391	8.8
10	2-Propanol, 2-methyl-	8.738	75-65-0	C4H10O	924	13361863	102.5
11	Methanol, TMS derivative	9.567	1825-61-2	C4H12OSi	911	6692393	51.4
12	Pentane, 2-methyl-	9.71	107-83-5	C6H14	809	145731	1.1
13	Silanol, trimethyl-	9.812	1066-40-6	C3H10OSi	906	89887970	689.7
14	Methyl vinyl ketone	10.193	78-94-4	C4H6O	876	1216322	9.3
15	1-Pentene, 2-methyl-	10.258	763-29-1	C6H12	775	148275	1.1
16	2,3-Butanedione	10.326	431-03-8	C4H6O2	678	77564	0.6
17	2-Butanone	10.442	78-93-3	C4H8O	777	194157	1.5
18	Propane, 2-ethoxy-2-methyl-	11.061	637-92-3	C6H14O	927	1538720	11.8
19	Isopropyl alcohol, TMS derivative	11.86	1825-64-5	C6H16OSi	861	435344	3.3
20	Ethane, 1,2-dichloro-	11.918	107-06-2	C2H4Cl2	887	170023	1.3
21	Disiloxane, hexamethyl-	12.356	107-46-0	C6H18OSi2	916	1511583	11.6
22	Butane, 2-methoxy-2-methyl-	12.479	994-05-8	C6H14O	817	62916	0.5
23	2-Pentanone	12.652	107-87-9	C5H10O	873	51521	0.4
24	Furan, 2,3-dihydro-4-methyl-	12.714	34314-83-5	C5H8O	772	46950	0.4
25	Pentanal	12.941	110-62-3	C5H10O	837	229192	1.8
26	Propane, 1,2-dichloro-	13.128	78-87-5	C3H6Cl2	794	248280	1.9
27	Heptane, 4-methyl-	14.516	589-53-7	C8H18	915	3711127	28.5
28	Toluene	14.659	108-88-3	C7H8	899	662141	5.1
29	4-Octene (Z)-	15.043	7642-15-1	C8H16	792	93885	0.7
30	Cyclopentanol, 2-methyl-, trans-	15.244	25144-04-1	C6H12O	757	171546	1.3
31	Cyclotrisiloxane, hexamethyl-	15.332	541-05-9	C6H18O3Si3	902	243678215	1869.8
32	Heptane, 2,4-dimethyl-	15.696	2213-23-2	C9H20	853	742792	5.7
33	2,4-Dimethyl-1-heptene	16.121	19549-87-2	C9H18	924	24002043	184.2
34	Trisiloxane, octamethyl-	16.462	107-51-7	C8H24O2Si3	882	1359009	10.4
35	Octane, 4-methyl-	16.564	2216-34-4	C9H20	823	429029	3.3
36	Cyclohexane, 1,3,5-trimethyl-, (1α,3α,5α)-	16.642	1795-27-3	C9H18	858	344659	2.6
37	4,4-Dimethyl-cyclohex-2-en-1-ol	16.815		C8H14O	686	49954	0.4
38	(E)-4-Chloro-3-methyl-3-hexen-2-one	16.89	105949-80-2	C7H11ClO	678	150599	1.2
39	Ethanone, 1-(1,2,2,3-tetramethylcyclopentyl)-, (1R-cis)-	17.172	59642-07-8	C11H20O	750	80693	0.6
40	o-Xylene	17.387	95-47-6	C8H10	872	83196	0.6
41	trisiloxane, 1,1,,15,5,5-hexamethyl-3-[(trimethylsilyl)oxy]	18.468		C9H28O3Si4	904	697399	5.4
42	Nonane, 2,6-dimethyl-	19.342	17302-28-2	C11H24	876	3797004	29.1
43	Octane, 3,3-dimethyl-	19.417	4110-44-5	C10H22	852	3901480	29.9
44	2-Decene, 7-methyl-, (Z)-	19.611	74630-23-2	C11H22	802	1158784	8.9
45	Carbonic acid, ethyl tridecyl ester	19.764		C16H32O3	670	70538	0.5
46	4-Undecene, (Z)-	19.805	821-98-7	C11H22	784	198383	1.5
47	Decane, 2,3,5,8-tetramethyl-	20.196	192823-15-7	C14H30	844	216023	1.7
48	2-Undecanethiol, 2-methyl-	20.597	10059-13-9	C12H26S	852	3102300	23.8
49	2-Undecanethiol, 2-methyl-	20.669	10059-13-9	C12H26S	853	3035920	23.3
50	Cyclotrisiloxane, hexamethyl-	20.995	541-05-9	C6H18O3Si3	934	63604615	488.1
	Other					10164943	78.0
					Total =	682593084	5237.7
				Response Factor =		26116766	200.4

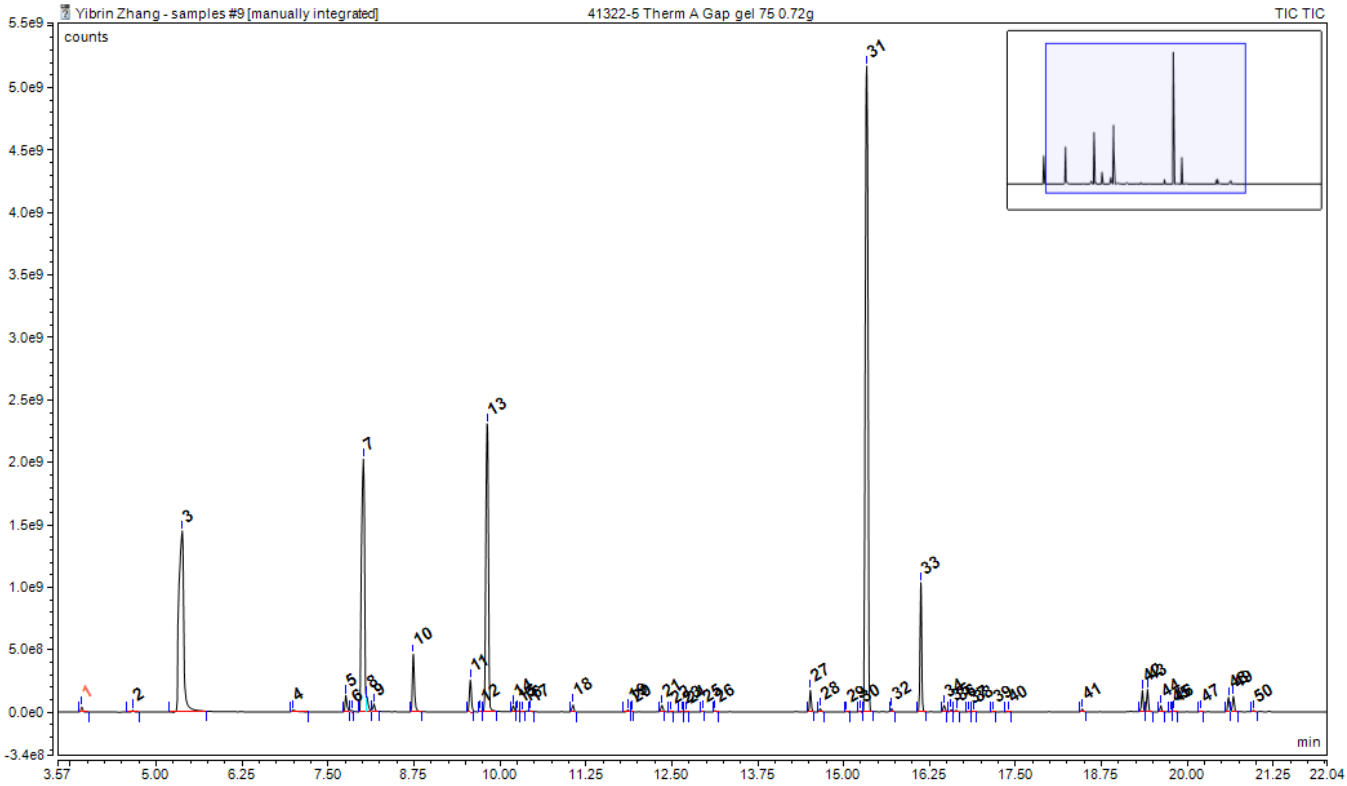


Figure B6. TIC for Therm-a-Gap 75 B: cryo-GC/MS headspace analysis. Peak indices correspond to compounds listed below in Table B6.

Table B6. Observed outgassing compounds from Therm-a-Gap 75 B: cryo-GC/MS headspace analysis. Peak indices correspond to peaks labeled in the chromatogram presented in Figure B6.

Peak #	ID	RT	CAS#	Formula	Match	Area	Approx Conc. (ppb)
1	Propene	3.915	115-07-1	C3H6	922	1096879	8.4
2	Chloromethane	4.66	74-87-3	CH3Cl	971	505496	3.9
3	Methyl Alcohol	5.377	67-56-1	CH4O	904	117062457	898.2
4	Ethanol	6.979	64-17-5	C2H6O	890	1186378	9.1
5	Acetone	7.755	67-64-1	C3H6O	849	4378123	33.6
6	2-Butene, 2-methyl-	7.843	513-35-9	C5H10	791	696323	5.3
7	Isopropyl Alcohol	8.013	67-63-0	C3H8O	934	103691997	795.7
8	Propane, 2-chloro-	8.064	75-29-6	C3H7Cl	913	3984536	30.6
9	1,3-Pentadiene, (E)-	8.166	2004-70-8	C5H8	933	2138665	16.4
10	2-Propanol, 2-methyl-	8.738	75-65-0	C4H10O	925	15583711	119.6
11	Methanol, TMS derivative	9.567	1825-61-2	C4H12OSi	925	8693282	66.7
12	Pentane, 2-methyl-	9.714	107-83-5	C6H14	842	204218	1.6
13	Silanol, trimethyl-	9.812	1066-40-6	C3H10OSi	908	101028201	775.2
14	Methyl vinyl ketone	10.193	78-94-4	C4H6O	878	1413613	10.8
15	1-Pentene, 2-methyl-	10.258	763-29-1	C6H12	833	274220	2.1
16	2,3-Butanedione	10.329	431-03-8	C4H6O2	895	78393	0.6
17	2-Butanone	10.441	78-93-3	C4H8O	949	364437	2.8
18	Propane, 2-ethoxy-2-methyl-	11.06	637-92-3	C6H14O	895	1875336	14.4
19	Isopropyl alcohol, TMS derivative	11.863	1825-64-5	C6H16OSi	845	632212	4.9
20	Ethane, 1,2-dichloro-	11.918	107-06-2	C2H4Cl2	895	221809	1.7
21	Disiloxane, hexamethyl-	12.356	107-46-0	C6H18OSi2	898	1759054	13.5
22	Butane, 2-methoxy-2-methyl-	12.482	994-05-8	C6H14O	809	82089	0.6
23	2-Pentanone	12.652	107-87-9	C5H10O	828	67208	0.5
24	Furan, 2,3-dihydro-4-methyl-	12.713	34314-83-5	C5H8O	837	94357	0.7
25	Pentanal	12.945	110-62-3	C5H10O	827	271289	2.1
26	Propane, 1,2-dichloro-	13.128	78-87-5	C3H6Cl2	830	376785	2.9
27	Heptane, 4-methyl-	14.516	589-53-7	C8H18	917	4714162	36.2
28	Toluene	14.662	108-88-3	C7H8	892	889969	6.8
29	4-Octene (Z)-	15.043	7642-15-1	C8H16	819	147949	1.1
30	Cyclopentanol, 2-methyl-, trans-	15.244	25144-04-1	C6H12O	792	350543	2.7
31	Cyclotrisiloxane, hexamethyl-	15.336	541-05-9	C6H18O3Si3	897	237240849	1820.4
32	Heptane, 2,4-dimethyl-	15.7	2213-23-2	C9H20	844	895226	6.9
33	2,4-Dimethylhep-1-ene	16.121		C9H18	917	29153322	223.7
34	Trisiloxane, octamethyl-	16.461	107-51-7	C8H24O2Si3	874	1622280	12.4
35	Octane, 4-methyl-	16.563	2216-34-4	C9H20	819	537466	4.1
36	Cyclohexane, 1,3,5-trimethyl-	16.642	1839-63-0	C9H18	857	451267	3.5
37	4,4-Dimethyl-cyclohex-2-en-1-ol	16.819		C8H14O	772	80457	0.6
38	(E)-4-Chloro-3-methyl-3-hexen-2-one	16.893	105949-80-2	C7H11ClO	668	215987	1.7
39	Ethanone, 1-(1,2,2,3-tetramethylcyclopentyl)-, (1R-cis)-	17.172	59642-07-8	C11H20O	753	112441	0.9
40	o-Xylene	17.39	95-47-6	C8H10	871	122694	0.9
41	trisiloxane, 1,1,,15,5,5-hexamethyl-3-[(trimethylsilyl)ox	18.472		C9H28O3Si4	882	776955	6.0
42	Nonane, 2,6-dimethyl-	19.346	17302-28-2	C11H24	874	4859808	37.3
43	Octane, 3,3-dimethyl-	19.42	4110-44-5	C10H22	857	5104363	39.2
44	2-Decene, 7-methyl-, (Z)-	19.614	74630-23-2	C11H22	801	1455153	11.2
45	Carbonic acid, ethyl tridecyl ester	19.767		C16H32O3	671	87067	0.7
46	4-Undecene, (Z)-	19.805	821-98-7	C11H22	757	325449	2.5
47	Decane, 2,3,5,8-tetramethyl-	20.196	192823-15-7	C14H30	835	276999	2.1
48	2-Undecanethiol, 2-methyl-	20.601	10059-13-9	C12H26S	847	3257564	25.0
49	2-Undecanethiol, 2-methyl-	20.669	10059-13-9	C12H26S	873	3670798	28.2
50	Decane, 2,3,5,8-tetramethyl-	20.961	192823-15-7	C14H30	806	400194	3.1
	Other					9774382	75.0
					Total =	674284411	5173.9
				Response Factor =		26116766	200.4

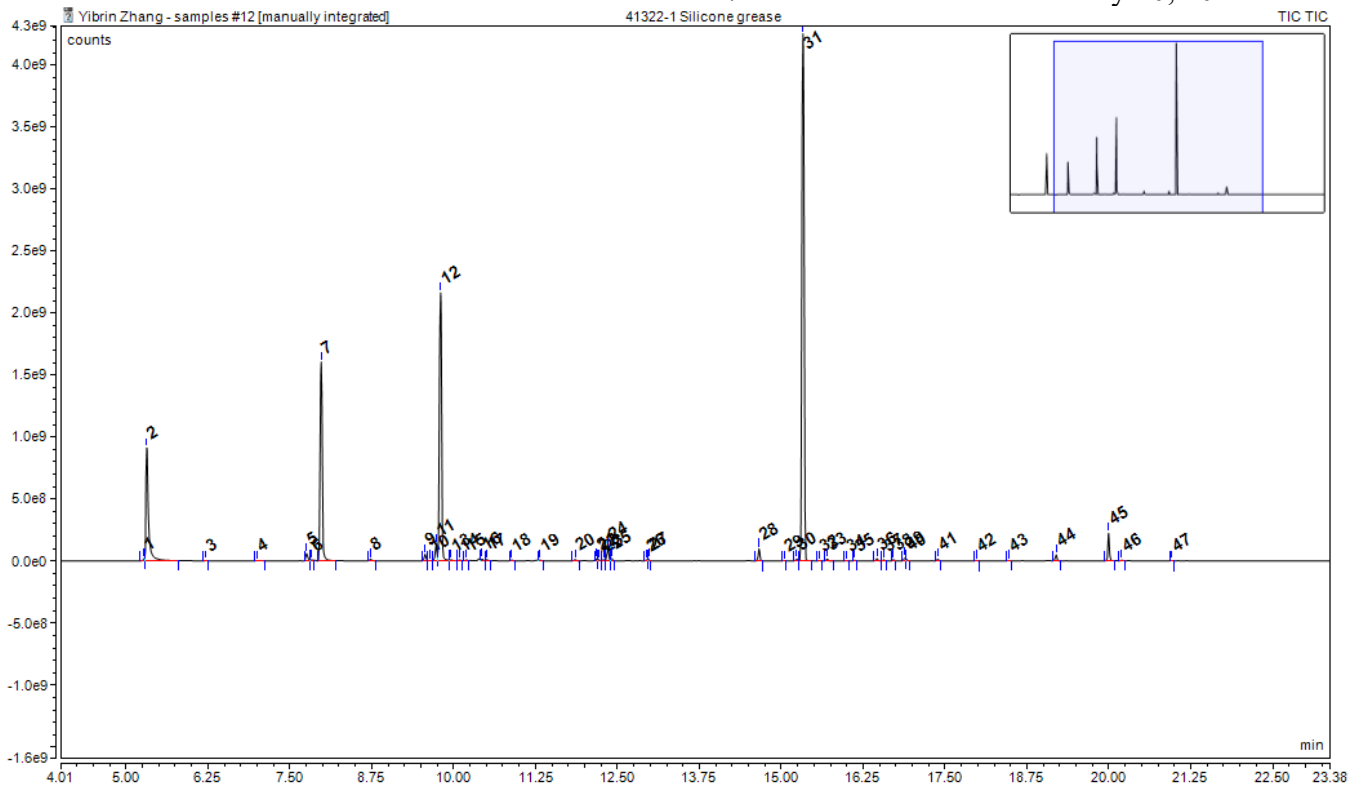


Figure B7. TIC for silicone grease A: cryo-GC/MS headspace analysis. Peak indices correspond to compounds listed below in Table B7.

Table B7. Observed outgassing compounds from silicone grease A: cryo-GC/MS headspace analysis. Peak indices correspond to peaks labeled in the chromatogram presented in Figure B7.

Peak #	ID	RT	CAS#	Formula	Match	Area	Approx Conc. (ppb)
1	Acetaldehyde	5.272	75-07-0	C2H4O	911	628959	4.8
2	Methyl Alcohol	5.316	67-56-1	CH4O	899	43548742	334.2
3	Benzene, 1-chloro-2-fluoro-	6.221	348-51-6	C6H4ClF	537	114222	0.9
4	Ethanol	6.996	64-17-5	C2H6O	846	252824	1.9
5	Acetone	7.755	67-64-1	C3H6O	942	2033944	15.6
6	Propanal	7.836	75-56-9	C3H6O	843	317685	2.4
7	Isopropyl Alcohol	7.979	67-63-0	C3H8O	933	63718635	488.9
8	2-Propanol, 2-methyl-	8.731	75-65-0	C4H10O	845	552049	4.2
9	Methanol, TMS derivative	9.564	1825-61-2	C4H12OSi	918	1802365	13.8
10	Butane, 2,3-dimethyl-	9.639	79-29-8	C6H14	811	75779	0.6
11	Ethylene, 1,2-dichloro-, (Z)-	9.734	156-59-2	C2H2Cl2	955	3941220	30.2
12	Silanol, trimethyl-	9.802	1066-40-6	C3H10OSi	916	87701693	673.0
13	2-Butenal, (E)-	9.962	123-73-9	C4H6O	835	258820	2.0
14	Pentane, 3-methyl-	10.094	96-14-0	C6H14	886	224328	1.7
15	Methyl vinyl ketone	10.193	78-94-4	C4H6O	897	200664	1.5
16	2-Butanone	10.431	78-93-3	C4H8O	936	466521	3.6
17	2-Ethyl-oxetane	10.506		C5H10O	865	331407	2.5
18	Ethyl Acetate	10.884	141-78-6	C4H8O2	856	235126	1.8
19	Cyclopentane, methyl-	11.319	96-37-7	C6H12	821	241768	1.9
20	Isopropyl alcohol, TMS derivative	11.856	1825-64-5	C6H16OSi	858	390903	3.0
21	Hexane, 2-methyl-	12.183	591-76-4	C7H16	836	618424	4.7
22	Cyclohexane	12.21	110-82-7	C6H12	858	285085	2.2
23	1-Hexene, 5-methyl-	12.288	3524-73-0	C7H14	786	375606	2.9
24	Disiloxane, hexamethyl-	12.356	107-46-0	C6H18OSi2	925	3308903	25.4
25	Hexane, 3-methyl-	12.411	589-34-4	C7H16	907	767488	5.9
26	Pentanal	12.941	110-62-3	C5H10O	850	253323	1.9
27	Heptane	12.975	142-82-5	C7H16	890	454885	3.5
28	Toluene	14.659	108-88-3	C7H8	915	2726552	20.9
29	Cyclopropane, 1-ethyl-2-pentyl-	15.043	62238-08-8	C10H20	802	70803	0.5
30	Hexane, 2,4-dimethyl-	15.237	589-43-5	C8H18	804	554002	4.3
31	Cyclotrisiloxane, hexamethyl-	15.332	541-05-9	C6H18O3Si3	918	175966251	1350.2
32	Hexane, 2,3,5-trimethyl	15.577	1069-53-0	C9H20	780	57909	0.4
33	Hexane, 2,3,4-trimethyl	15.7	921-47-1	C9H20	848	517925	4.0
34	Cyclohexene, 3,3,5-trimethyl-	15.992	503-45-7	C9H16	824	45835	0.4
35	2,4-Dimethyl-1-heptene	16.121	19549-87-2	C9H18	843	173069	1.3
36	Trisiloxane, octamethyl-	16.461	107-51-7	C8H24O2Si3	857	646111	5.0
37	Octane, 4-methyl-	16.563	2216-34-4	C9H20	838	273092	2.1
38	Ethylbenzene	16.713	100-41-4	C8H10	915	331440	2.5
39	Benzene, 1,3-dimethyl-	16.883	108-38-3	C8H10	947	871357	6.7
40	o-Xylene	16.91	95-47-6	C8H10	921	354737	2.7
41	p-Xylene	17.39	106-42-3	C8H10	910	510544	3.9
42	Benzene, 1-ethyl-2-methyl-	17.978	611-14-3	C9H12	862	144613	1.1
43	trisiloxane, 1,1,1,5,5,5-hexamethyl-3-[(trimethylsilyl)oxy]-	18.471		C9H28O3Si4	887	125157	1.0
44	Decane	19.196	124-18-5	C10H22	890	1565598	12.0
45	Cyclohexene, 1-methyl-5-(1-methylethenyl)-, (R)-	19.995	1461-27-4	C10H16	886	5905150	45.3
46	Dodecane, 2,6,11-trimethyl-	20.196	31295-56-4	C15H32	846	177449	1.4
47	Decane, 2,3,5,8-tetramethyl-	20.961	192823-15-7	C14H30	803	134081	1.0
	Other					3840476	29.5
					Total =	408093516	3131.4
				Response Factor =		26116766	200.4

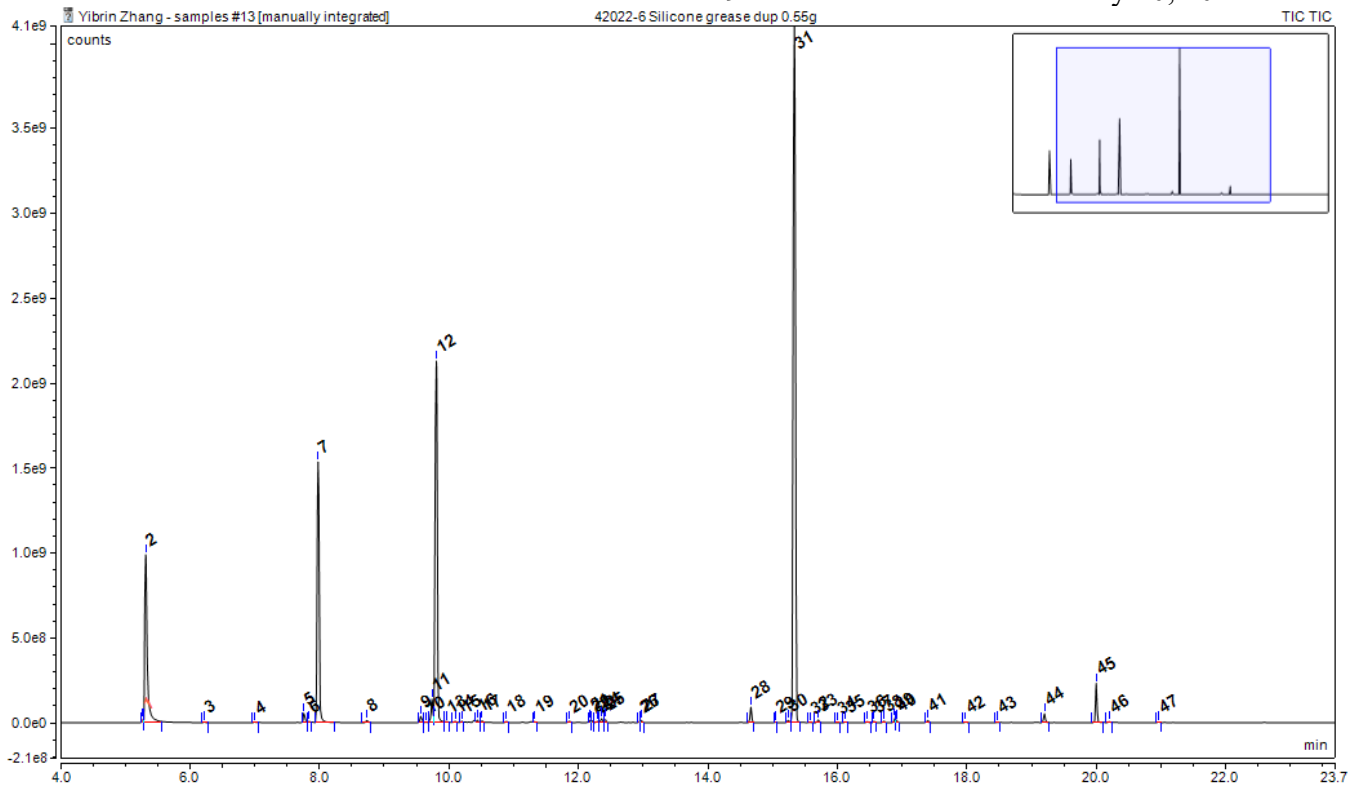


Figure B8. TIC for silicone grease B: cryo-GC/MS headspace analysis. Peak indices correspond to compounds listed below in Table B8..

Table B8. Observed outgassing compounds from silicone grease B: cryo-GC/MS headspace analysis. Peak indices correspond to peaks labeled in the chromatogram presented in Figure B8.

Peak #	ID	RT	CAS#	Formula	Match	Area	Approx Conc. (ppb)
1	Acetaldehyde	5.27	75-07-0	C2H4O	932	560064	4.3
2	Methyl Alcohol	5.32	67-56-1	CH4O	952	44458334	341.1
3	Benzene, 1-chloro-2-fluoro-	6.22	348-51-6	C6H4ClF	546	114752	0.9
4	Ethanol	7.00	64-17-5	C2H6O	850	146527	1.1
5	Acetone	7.76	67-64-1	C3H6O	936	1649368	12.7
6	Propanal	7.84	75-56-9	C3H6O	853	69104	0.5
7	Isopropyl Alcohol	7.98	67-63-0	C3H8O	937	58263649	447.1
8	2-Propanol, 2-methyl-	8.73	75-65-0	C4H10O	802	445554	3.4
9	Methanol, TMS derivative	9.57	1825-61-2	C4H12OSi	881	1315930	10.1
10	Butane, 2,3-dimethyl-	9.64	79-29-8	C6H14	599	50531	0.4
11	Ethylene, 1,2-dichloro-, (Z)-	9.74	156-59-2	C2H2Cl2	953	3956040	30.4
12	Silanol, trimethyl-	9.81	1066-40-6	C3H10OSi	901	86514873	663.8
13	2-Butenal, (E)-	9.97	123-73-9	C4H6O	827	58710	0.5
14	Pentane, 3-methyl-	10.10	96-14-0	C6H14	850	206976	1.6
15	Methyl vinyl ketone	10.20	78-94-4	C4H6O	884	194826	1.5
16	2-Butanone	10.44	78-93-3	C4H8O	933	356609	2.7
17	2-Ethyl-oxetane	10.51		C5H10O	901	312066	2.4
18	Ethyl Acetate	10.89	141-78-6	C4H8O2	877	204839	1.6
19	Cyclopentane, methyl-	11.33	96-37-7	C6H12	834	124859	1.0
20	Isopropyl alcohol, TMS derivative	11.86	1825-64-5	C6H16OSi	782	331214	2.5
21	Hexane, 2-methyl-	12.19	591-76-4	C7H16	845	461618	3.5
22	Cyclohexane	12.20	110-82-7	C6H12	862	245295	1.9
23	1-Hexene, 5-methyl-	12.29	3524-73-0	C7H14	788	168796	1.3
24	Disiloxane, hexamethyl-	12.36	107-46-0	C6H18OSi2	904	666595	5.1
25	Hexane, 3-methyl-	12.41	589-34-4	C7H16	875	528641	4.1
26	Pentanal	12.95	110-62-3	C5H10O	800	231538	1.8
27	Heptane	12.98	142-82-5	C7H16	885	429666	3.3
28	Toluene	14.67	108-88-3	C7H8	925	2572124	19.7
29	Cyclopropane, 1-ethyl-2-pentyl-	15.05	62238-08-8	C10H20	779	77441	0.6
30	Hexane, 2,4-dimethyl-	15.24	589-43-5	C8H18	793	490925	3.8
31	Cyclotrisiloxane, hexamethyl-	15.34	541-05-9	C6H18O3Si3	923	171356941	1314.9
32	Hexane, 2,3,5-trimethyl	15.58	1069-53-0	C9H20	634	52891	0.4
33	Hexane, 2,3,4-trimethyl-	15.70	921-47-1	C9H20	851	506464	3.9
34	Cyclohexene, 3,3,5-trimethyl-	16.00	503-45-7	C9H16	530	17719	0.1
35	2,4-Dimethyl-1-heptene	16.13	19549-87-2	C9H18	824	166084	1.3
36	Trisiloxane, octamethyl-	16.46	107-51-7	C8H24O2Si3	821	240082	1.8
37	Octane, 4-methyl-	16.57	2216-34-4	C9H20	812	247539	1.9
38	Ethylbenzene	16.72	100-41-4	C8H10	931	308100	2.4
39	Benzene, 1,3-dimethyl-	16.89	108-38-3	C8H10	947	779392	6.0
40	o-Xylene	16.92	95-47-6	C8H10	920	311274	2.4
41	p-Xylene	17.39	106-42-3	C8H10	920	423077	3.2
42	Benzene, 1-ethyl-2-methyl-	17.98	611-14-3	C9H12	859	146583	1.1
43	trisiloxane, 1,1,1,5,5,5-hexamethy	18.47		C9H28O3Si4	884	90902	0.7
44	Decane	19.20	124-18-5	C10H22	888	1635672	12.6
45	Cyclohexene, 1-methyl-5-(1-meth	20.00	1461-27-4	C10H16	889	6134745	47.1
46	Dodecane, 2,6,11-trimethyl-	20.20	31295-56-4	C15H32	787	181179	1.4
47	Decane, 2,3,5,8-tetramethyl-	20.97	192823-15-7	C14H30	785	163158	1.3
	Other					10492786	80.5
					Total =	398462052	3057.5
				Response Factor =		26116766	200.4

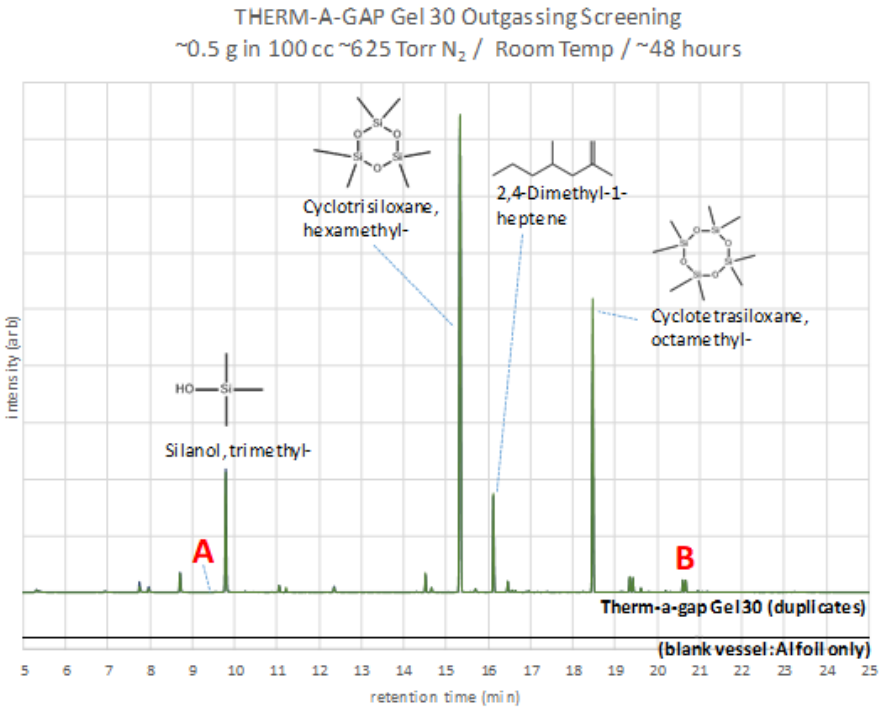
Appendix C. Original December, 2021 Outgassing study of Therm-a Gap Gel 30 (Summary Slides)

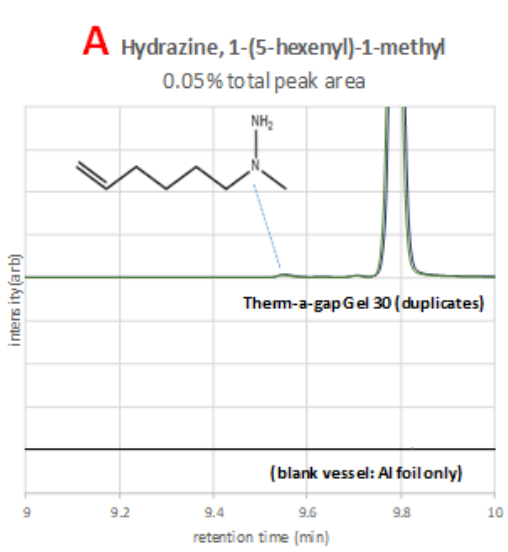
Outgassing Characterization: Therm-a-Gap Gel 30

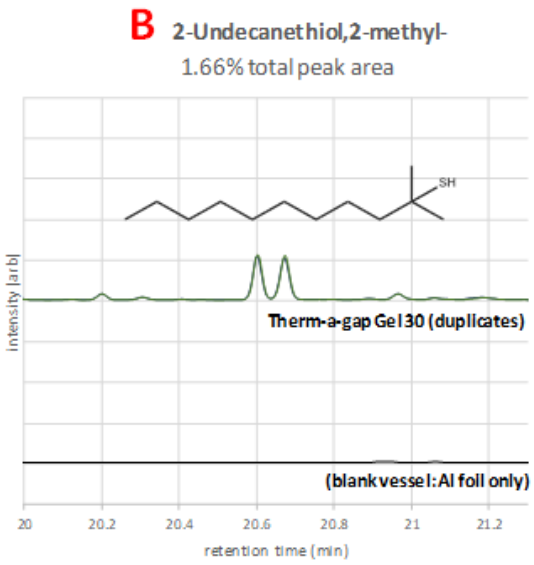
Jason Brown and Ray Fuentes
SNL-NM 12/06/2021

- Headspace analysis (volatiles): ~0.5 g Gel 30 administered to Al foil and sealed in stainless steel vessel (~100 cc, verified clean); backfilled with dry N_2. (Duplicate samples prepared.)
- Vessel held at room temperature for ~48 hours before undergoing headspace analysis using cryo-GC/MS. (Samples run in duplicate)
- Blank vessel also prepared (Al foil only)

- Samples yielded excellent results (good chromatography and repeatability; see TICs)
- Unsurprisingly, siloxanes/silanol largest contributors (~83% total peak area)
- Complex mix of minor organics, most appear to be innocuous (other materials SMEs should review)
- 2 potential compounds of interest noted; potentially reactive species (A, B; see next slide)

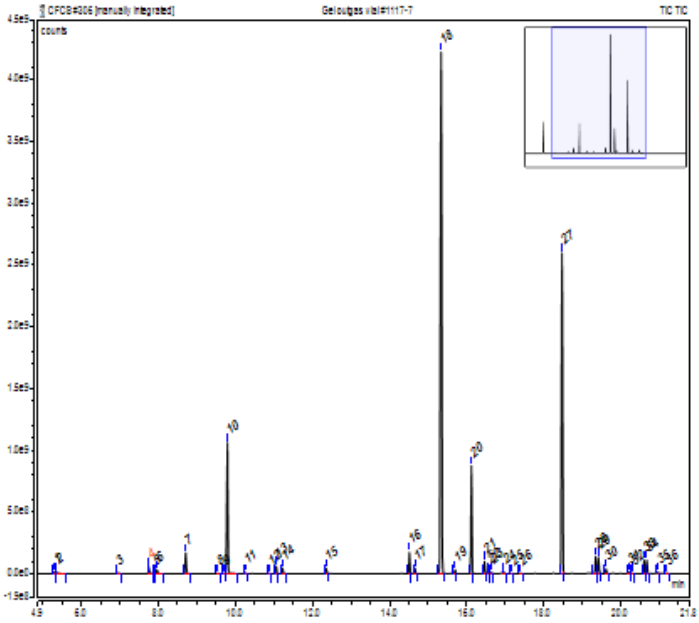






- 2 potential compounds of interest noted; potentially reactive species (labeled A, B on previous slide)

All Peak IDs in Headspace Analysis of Therm-a-Gap Gel 30



Total Ion Chromatogram (TIC): Therm-a-Gap Gel 30

Peak	Compound	RT (min)	Peak Area	CAS #
1	2-Butene	5.309	0.20%	107-01-7
2	Methyl Alcohol	5.36	0.23%	67-56-1
3	Ethanol	6.925	0.13%	64-17-5
4	Acetone	7.748	0.49%	67-64-1
5	Isobutane	7.887	0.03%	75-28-5
6	Isopropyl Alcohol	7.965	0.31%	67-63-0
7	2-Propanol, 2-methyl-	8.707	1.46%	75-65-0
8	Hydrazine, 1-(5-hexenyl)-1-methyl-	9.547	0.05%	53907-78-1
9	Butane, 2,3-dimethyl-	9.703	0.02%	79-29-8
10	Silanol, trimethyl-	9.788	9.25%	1066-40-6
11	1-Pentene, 2-methyl-	10.251	0.07%	763-29-1
12	3-Penten-2-ol	10.877	0.03%	1569-50-2
13	Propane, 2-ethoxy-2-methyl-	11.054	0.50%	637-92-3
14	Oxetane, 2,2-dimethyl-	11.217	0.38%	6245-99-4
15	Disiloxane, hexamethyl-	12.349	0.38%	107-46-0
16	Heptane, 4-methyl-	14.512	1.25%	589-53-7
17	Toluene	14.659	0.32%	108-88-3
18	Cyclotrisiloxane, hexamethyl-	15.336	47.31%	541-05-9
19	Heptane, 2,4-dimethyl-	15.699	0.29%	2213-23-2
20	2,4-Dimethyl-1-heptene	16.121	6.67%	19549-87-2
21	Trisiloxane, octamethyl-	16.461	0.76%	107-51-7
22	Octane, 4-methyl-	16.563	0.13%	2216-34-4
23	Cyclohexane, 1,3,5-trimethyl-	16.642	0.14%	1839-63-0
24	4-Cyclohexyl-3-methylphenol, TMS	16.961	0.09%	
25	Ethanone, 1-(1,2,2,3-tetramethylcyclopentyl)-, (1R-cis)-	17.172	0.04%	59642-07-8
26	Benzene, 1,3-dimethyl-	17.39	0.07%	108-38-3
27	Cyclotetrasiloxane, octamethyl-	18.471	25.00%	556-67-2
28	Nonane, 2,6-dimethyl-	19.345	1.10%	17302-28-2
29	Nonane, 2,6-dimethyl-	19.42	0.98%	17302-28-2
30	4-Decene, 7-methyl-, (E)-	19.614	0.31%	62338-48-1
31	Heptadecane, 2,6,10,14-tetramethyl-	20.199	0.12%	18344-37-1
32	Heptadecane, 2,6-dimethyl-	20.305	0.05%	54105-67-8
33	2-Undecanethiol, 2-methyl-	20.6	0.83%	10059-13-9
34	2-Undecanethiol, 2-methyl-	20.672	0.83%	10059-13-9
35	Heptadecane, 2,6,10,14-tetramethyl-	20.968	0.12%	18344-37-1
36	Decane, 2,4,6-trimethyl-	21.185	0.07%	62108-27-4