

Organic Gas Speciation Profile for Structural, Open-Burning, and Vehicle Fire Emissions

OG1492–OG1496

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Introduction

Structural fires, vehicle fires, and related open-burning sources emit complex mixtures of organic gases from combustion of wood, paper, plastics, synthetic polymers, fuels, and other built-environment materials. These emissions may occur during individual fire events and can also be relevant to open-burning and refuse-related categories. Because these source types involve heterogeneous fuels and variable burning conditions, their emissions can include a broad range of reactive and toxic organic compounds. Emission composition is also strongly influenced by combustion phase (flaming versus smoldering), ventilation conditions, combustion temperature, and fuel-specific thermal decomposition pathways. These factors can affect both the mixture of emitted organic gases and their ozone-forming potential.

Previous profile assignments for these categories relied largely on a single surrogate profile rather than separate source- or material-specific profiles. In Yang (2018) [1], structural fires, automobile fires, and commercial or institutional open burning of refuse were represented using OG1476, a garbage burning profile. More recent work provides a better basis for source-specific profile development. Link et al. (2025) [2] reported controlled hood-calorimeter experiments using mixed residential-building surrogates across different sizes and packing densities, and Holder et al. (2023) [3] compiled available gas-phase measurements for vehicle fires.

The objective of this report is to update CARB's total organic gas (TOG) speciation profiles for structural fire, open-burning, and vehicle fire sources using recently available measurement data and related supporting literature. The updated profiles are intended to replace older surrogate assignments with more source-specific profiles in the CARB speciation database. The profiles discussed in this document are:

- OG1492: Structural Fire–Mixed Building Materials
- OG1493: Solid Waste/Refuse Burning
- OG1494: Cellulosic Material Burning
- OG1495: Synthetic Polymer Material Burning
- OG1496: Vehicle Fires

Data Sources and Methods

Reference datasets and measurement basis

Profiles for structural fire, open-burning, and vehicle fire sources were developed using a combination of source-specific and surrogate-based datasets. Structural and open-burning profiles were informed primarily by the laboratory combustion experiments reported by Link et al. (2025) [2], while vehicle fire emissions were represented using the literature compilation reported by Holder et al. (2023) [3].

Where source studies reported species-level emission factors, those data were converted to TOG speciation profiles by normalizing each species emission factor to the total measured organic gas emissions. The resulting normalized fractions represent the contribution of each species to TOG and provide a profile format suitable for use in the California Air Resources Board (CARB)'s speciation database.

Link et al. (2025)[2] conducted controlled combustion experiments using mixed residential building surrogates composed of approximately 70% combustible wood and 30% synthetic polymers. The study reported chemically resolved total NMOG emissions from these surrogate burns and also used positive matrix factorization to identify recurring composition factors associated with wood combustion, synthetic polymer combustion, and mixed fuel char. In this study, the total emissions data were used to represent mixed structural and open-burning conditions, while the PMF-resolved factor profiles were used to derive surrogate wood-rich, polymer-rich, and mixed-material composition profiles for inventory-facing source assignments.

Vehicle fire emissions were represented using the compilation reported by Holder et al. (2023) [3], which synthesized available measurements of gas-phase emissions from vehicle fire events reported in the literature. Since comprehensive and internally consistent vehicle-fire speciation datasets remain limited, this compilation was used as the best available basis for development of a vehicle fire TOG profile.

Fuel Selection

Speciation profiles for structural fire, open-burning, and related urban fire sources were derived primarily from the controlled combustion experiments reported by Link et al. (2025) [2]. All six surrogate configurations were burned under the same hood-calorimeter system, with surrogate size and packing density varied to examine ventilation and fuel-loading effects. The surrogate fuel mixture included gypsum board, untreated wood, oriented strand board, PVC, polyurethane, and ABS, with combustible mass composed of approximately 70% wood and 30% synthetic polymers.

To represent mixed-material structural fires, a structural fire profile was calculated as the average of the large-surrogate experiments reported by Link et al. (2025) [2], specifically the LL, LM, and LH tests representing low, medium, and high packing density conditions in the large-surrogate configurations. These experiments were used as a surrogate for structural fires involving mixed residential building materials.

For refuse or solid waste burning, a separate profile was derived as the average of the small-surrogate experiments (SL, SM, and SH), which represent combustion of mixed household materials. These experiments were used as a proxy for refuse or waste burning because they reflect combustion occurring in open environments with mixed residential materials.

Link et al. (2025)[2] also reported positive matrix factorization (PMF) results that resolved emissions associated with dominant material types present in the experiments. These PMF-resolved factors were used to develop material-specific surrogate profiles where direct source-specific measurements were not available. The wood PMF factor was used as the proxy profile for paper-based materials, while the synthetic polymer PMF factor was used as the proxy profile for plastic-based materials. Because the PMF-derived factors were based on Proton-Transfer-Reaction Mass Spectrometry (PTR-MS) non-methane organic gas (NMOG) measurements and therefore did not include methane, CH4 was incorporated from the corresponding combustion experiments so that the final profiles would represent total organic gas (TOG).

Vehicle fire emissions were represented using a composite profile derived from the literature synthesis reported by Holder et al. (2023), which compiled available measurements of organic gas emissions from vehicle fires across multiple studies. Because direct vehicle-fire speciation datasets remain limited and variable in experimental design, this profile was used as the best-available composite representation for automobile fire emissions in the inventory.

Treatment of unresolved masses and isomer splits

For the C2H4O2 signal, a 95:5 split between acetic acid and glycolaldehyde was applied to all applicable structural and open-burning profiles, OG1492 through OG1495. This split was based on the biomass-burning measurements reported by Hatch et al. (2015) [4], which support acetic acid as the dominant contributor to this unresolved formula group. The C2H4O2 mass was therefore removed from each applicable profile-specific lumped species and reassigned as 95% acetic acid and 5% glycolaldehyde in Table A3. OG1496 was unchanged because the vehicle-fire profile did not contain this unresolved C2H4O2 signal.

The source-reported formula groups labeled “chlorodioxin” and “chlorobenzofurans” were also reviewed following comments from CARB toxics staff. CATEF dioxin/furan congener fractions were evaluated as a possible further-speciation approach but were not applied. The Link et al. PTR-ToF-MS signals were assigned formulas C4H3ClO2 and C8H5ClO, respectively, whereas the PCDD/F congeners represented in CATEF have different formulas and substantially higher molecular weights. Applying CATEF congener fractions would therefore assign the measured PTR-ToF-MS mass to chemically different compounds. No corresponding AB2588 toxic-air-contaminant entries were identified for these low-molecular-weight formula groups. The signals were therefore retained within the applicable profile-specific lumped species and documented in Table A4 rather than being assigned to PCDD/F congeners.

PTR-MS measurements may also underrepresent certain semi-volatile or low-volatility organic compounds that partition to particles or sampling surfaces during combustion sampling. As a result, the gas-phase TOG profiles may not fully represent all organic vapors relevant to secondary organic aerosol (SOA) formation.

Additional harmonization was required for the PMF-resolved factors reported by Link et al. (2025) [2]. Because those factors were reported on an NMOG basis and did not include methane, CH4 from the corresponding combustion experiments was incorporated so that the final surrogate profiles would be represented on a TOG basis consistent with the CARB speciation database. The resulting profiles therefore combine the chemically resolved PMF-based composition information with total-organic-gas normalization needed for inventory application. Because PMF factors represent statistically resolved compositional patterns rather than direct source measurements, the resulting material-specific profiles should be interpreted as surrogate approximations of dominant combustion signatures.

Development of TOG Speciation Profiles from Emission Factors

For each profile, species-level emission factors or composition factors were converted to TOG weight fractions after applying the supported compound assignments and incorporating methane where required. The resulting fractions were expressed as percent of TOG and rounded to four decimal places. Final profiles were checked to sum to 100.0000%.

Results and Discussion

Table 1. Summary of newly developed TOG speciation profiles (OG1492–OG1496), including source categories, reference datasets, and profile derivation methods.

Profile ID	Profile Name	Source Category	Reference	Proxy / Averaging Description
OG1492	Structural Fire–Mixed Building Materials	Structural Fires	Link et al. (2025) [2]	Average of large-surrogate experiments LL, LM, and LH representing mixed residential building materials in the large-surrogate configurations

Profile ID	Profile Name	Source Category	Reference	Proxy / Averaging Description
OG1493	Solid Waste / Refuse Burning	Waste Combustion	Link et al. (2025) [2]	Average of small-surrogate experiments SL, SM, and SH representing mixed residential materials in the small-surrogate configurations
OG1494	Cellulosic Material Burning	Agricultural / Waste Materials	Link et al. (2025) [2]	Hybrid surrogate profile based on the wood PMF factor identified in the Link et al. PMF analysis, applied to cellulosic materials, with methane incorporated from small-scale combustion measurements
OG1495	Synthetic Polymer Material Burning	Agricultural / Waste Materials	Link et al. (2025) [2]	Hybrid profile derived from the synthetic polymer PMF factor from Link et al., with methane emissions incorporated from small-scale combustion measurements
OG1496	Vehicle Fires	Vehicle Fires	Holder et al. (2023) [3]	Composite vehicle-fire profile compiled from literature measurements of burning passenger vehicles and vehicle components

Chemical Composition

Differences in Chemical Composition of New and Old Structural and Open-Burning Profiles

The updated structural fire and related open-burning profiles (OG1492–OG1495) show substantially expanded chemical detail relative to the previous surrogate profile, OG1476 (see Table 2). Across the four updated profiles, the average ROG fraction was 85.7 ± 2.9% of TOG, with average CH4, NMHC, and OVOC fractions of 13.2 ± 2.7%, 47.8 ± 7.3%, and 23.0 ± 10.8%, respectively. By comparison, OG1476 had a ROG fraction of 86.1% of TOG, with CH4, NMHC, and OVOC fractions of 13.94%, 11.12%, and 15.84%, respectively.

Methanol and formic acid were not found in the new OG1493 compared to legacy profile, OG1476. Their absence should not be interpreted to mean that these compounds cannot occur in refuse-burning emissions. Small oxygenated compounds can vary with fuel mixture, ventilation, residence time, and combustion efficiency. Guérette et al. (2018) [5] showed that methanol and formic acid emission factors depend on modified combustion efficiency. Therefore, the absence of these species in OG1493 was treated as a source-condition and measurement uncertainty

The updated structural and open-burning profiles also provide much broader compound-level representation than the previous surrogate profile. They contain 174 to 175 explicitly represented ROG compounds, 30 to 32 NMHC compounds, and 74 OVOC compounds, compared with 9 ROG compounds, 3 NMHC compounds, and 4 OVOC compounds in OG1476. This increase reflects the improved chemical resolution of the newer measurement datasets and the use of material-resolved surrogate profiles rather than a single generic garbage-burning assignment. The primary improvement is not only the larger number of listed compounds, but the substantially improved representation of chemically resolved reactive mass and functional-group diversity, including oxygenated, aromatic, nitrile, and halogenated organic compounds that were poorly represented in the previous surrogate profile.

Vehicle Fire Profile

The updated vehicle fire profile (OG1496) also provides a more source-relevant and chemically explicit representation than the previous surrogate profile, OG1476, which had previously been used for automobile fires. OG1496 has a ROG fraction of 67.9% of TOG, with CH4, NMHC, and OVOC fractions of 29.10%, 11.46%, and 18.49%, respectively, compared with 86.1%, 13.94%, 11.12%, and 15.84% in OG1476.

Although the vehicle fire profile has a lower overall ROG fraction than OG1476, it includes more explicit compound-level information, with 14 represented ROG compounds, 7 NMHC compounds, and 5 OVOC compounds, compared with 9, 3, and 4, respectively, in the previous surrogate profile. These results indicate that OG1496 provides a more source-specific representation of automobile fire emissions than the earlier generic garbage-burning assignment.

Vehicle fire emissions remain comparatively under-characterized, and OG1496 should be considered a provisional composite profile pending availability of more comprehensive controlled measurement datasets. Real-world vehicle fires can vary with vehicle age, fuel type, tire and plastic involvement, catalytic converter condition, fuel tank involvement, and electric-vehicle battery contributions.

Table 2. Comparison of chemical composition metrics between updated fire-related TOG profiles (OG1492–OG1496) and the previously used profile (OG1476). Here composition is broadly summarized by Reactive Organic Gases (ROG), methane, Non-Methane Hydrocarbons (NMHC), and Oxygenated Volatile Organic Compounds (OVOC).

Parameter	Previous profile (OG1476)	Structural and open-burning new (OG1492–OG1495)	Vehicle fire new (OG1496)
ROG fraction (% of TOG)	86.1	85.7 ± 2.9	67.9
CH4 fraction (% of TOG)	13.94	13.2 ± 2.7	29.1
NMHC fraction (% of TOG)	11.12	47.8 ± 7.3	11.46
OVOC fraction (% of TOG)	15.84	23.0 ± 10.8	18.49
Number of ROG compounds	9	174–175	14
Number of NMHC compounds	3	30–32	7
Number of OVOC compounds	4	74	5
Number of toxic species†	7	38-39	11

Differences among the New Structural and Open-Burning Profiles

The four updated structural and open-burning profiles also differ meaningfully from one another. OG1492, which represents mixed building materials burned in a structural fire, has the highest OVOC fraction among the four profiles (35.00% of TOG), indicating a comparatively greater contribution from oxygenated combustion products. OG1493, representing refuse/open-burning surrogate, has a higher CH4 fraction (15.98% of TOG) and a somewhat lower ROG fraction than OG1492, while still remaining rich in hydrocarbons and oxygenated compounds. OG1494, the cellulosic surrogate profile, is dominated by acetylene, methane, and ethene and shows a composition broadly similar to OG1493 but with a larger contribution from other identified heteroatom-containing species. In contrast, OG1495, the synthetic polymer surrogate profile, is the most hydrocarbon-rich of the four, with the highest NMHC fraction (58.03% of TOG), the lowest OVOC fraction (8.84% of TOG), and the highest ROG fraction (89.20% of TOG). These differences indicate that the updated profiles capture clear variability across mixed structural materials, refuse burning, cellulosic materials, and synthetic polymers, rather than representing all open-burning-related sources with a single generic surrogate profile.

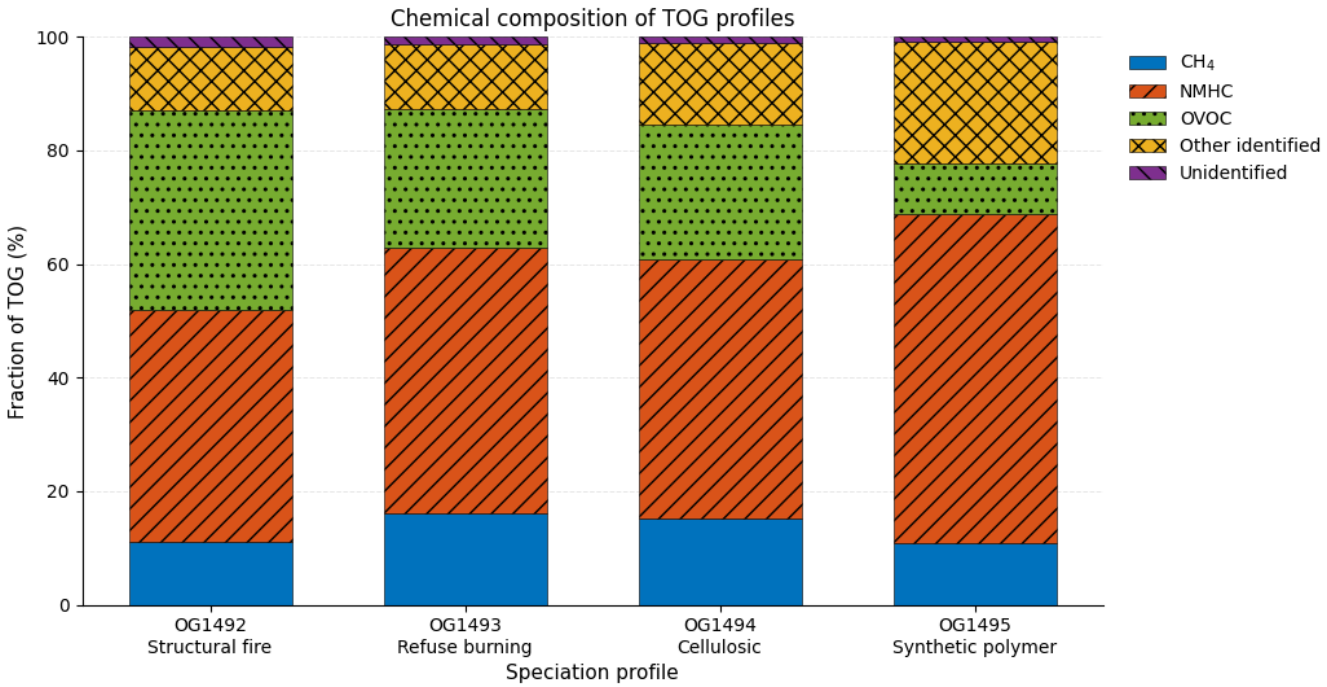


Figure 1. Composition summary of updated structural and open-burning TOG profiles (OG1492–OG1495)

Implications For Emission Inventory and Modeling

Representation of toxic air contaminants

The updated structural, open-burning, and vehicle fire profiles substantially expand the representation of toxic air contaminants relative to the previous CARB surrogate profile, OG1476. The updated structural and open-burning profiles contain more than 37 explicitly represented toxic species per profile, compared with 7 in OG1476. The updated vehicle fire profile contains 11 toxic species, which is also higher than the previous surrogate profile.

This increase reflects both the improved chemical resolution of the newer datasets and the use of source-relevant, material-resolved surrogate profiles in place of a single generic garbage-burning assignment. In addition to commonly represented compounds such as formaldehyde, the updated profiles explicitly include additional toxic compounds such as acrolein, vinyl chloride, pyridine, acrylonitrile, guaiacol, styrene, benzaldehyde, benzofuran, furfural, methyl methacrylate, and naphthalene. The broader inclusion of these compounds provides a more realistic basis for toxic emissions characterization and downstream health-oriented analyses.

The updated profiles also improve the treatment of source-reported chlorinated formula groups. The source data reported C4H3ClO2 and C8H5ClO signals using non-standard group labels. CATEF congener fractions were not applied because these formula groups do not correspond to the higher-molecular-weight PCDD/F congeners represented in CATEF. The unresolved groups remain within the profile-specific lumped species and are not counted as confirmed PCDD/F toxic species. Separate SAPRC-oriented isomer splits may indicate potential toxic constituents, but these tentative modeling assignments are not treated as source-resolved toxics in this report.

Ozone formation potential

The updated profiles also increase the ozone formation potential (OFP) assigned to combustion emissions in the inventory. OFP was calculated as $OFP = \sum_1^i f_i \times MIR_i$. Where f_i is the fractional abundance of species i in TOG and MIR_i is its Maximum Incremental Reactivity (MIR) – a scale used to estimate reactivity to form ozone[6]. However, MIR-based OFP estimates represent incremental ozone formation under high-NOx urban photochemical conditions and should be interpreted as a relative ozone-reactivity metric rather than a direct estimate of secondary organic aerosol formation or total secondary-pollutant production.

For the source groups evaluated here, the mean profile-level OFP of the updated structural and open-burning profiles is 2.61 ± 0.33 g O3 per g TOG, compared with 1.32 g O3 per g TOG for the previous surrogate profile, OG1476. The updated vehicle fire profile has an

OFP of 1.85 g O3 per g TOG, compared with 1.32 g O3 per g TOG previously assigned using OG1476. OG1476 was previously used for refuse burning, structural fires, and automobile fires.

Using the 2023 inventory TOG emissions shown in Table 3, the updated profiles increase estimated ozone forming potential from 10.1 to 20.0 tons/day for structural and related open-burning sources and from 0.35 to 0.49 tons/day for vehicle fires. Summed across these categories, total estimated ozone formation increases from 10.45 to 20.45 tons/day, an increase of 10.0 tons/day or 96%. This increase reflects improved chemical representation, with more mass assigned to explicitly resolved reactive compounds, including oxygenated and other highly reactive species that contribute strongly to ozone formation.

In addition to ozone formation, the updated profiles may affect modeled secondary organic aerosol formation because combustion emissions from structural and material burning contain aromatic and oxygenated organic compounds, as well as other organic species that may act as SOA precursors.

Table 3. Change in ozone-forming potential and estimated ozone formation for structural, open-burning, and vehicle fire emissions using updated TOG speciation profiles.

Metric	Old structural fire profile	New structural fire profiles	Vehicle fire old profile	Vehicle fire new profile	Total with old profiles	Total with new profiles
TOG emissions (tons/day)	7.65	7.65	0.262	0.262	7.91	7.91
Mean OFP (g O3/g TOG)	1.32	2.61 ± 0.33 (2.28–2.94)	1.32	1.85		
Estimated ozone formation (tons/day)	10.10	19.96	0.35	0.49	10.45	20.45
Change (tons/day)	—	9.86		0.14		10.00
% change	—	97.6%		40.0%		95.7%

Uncertainty and limitations

The updated profiles provide improved source-specific chemical representation relative to the previous surrogate assignment; however, several uncertainties remain. Structural-fire and open-burning emissions are influenced by fuel composition, combustion phase, ventilation, combustion temperature, and material-specific thermal decomposition pathways.

The surrogate materials used in the source studies represent broad categories of residential combustible materials and included wood, gypsum board, PVC, polyurethane, and ABS; however, they may not capture the full variability of real-world fires. Actual structural fires may differ due to building age, furnishings, the amount and configuration of PVC-containing materials, flame retardants, electronics, and emerging combustion sources such as lithium-ion batteries.

The material-specific profiles derived from PMF-resolved factors should be interpreted as surrogate approximations of dominant combustion signatures rather than direct measurements from isolated fuels. In addition, PTR-MS-based measurements may underrepresent some low-volatile and semi-volatile organic compounds that partition to particles or sampling surfaces.

Vehicle-fire emissions remain comparatively under-characterized, and the vehicle-fire profile should be considered provisional pending availability of more comprehensive controlled measurement datasets.

References

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Appendix

Table A1. Mapping of EIC/SCC codes to updated fire-related TOG speciation profiles added in this work.

EIC/SCC	Category	Sub-Category 1	Sub-Category 2	Sub-Category 3	New OG Profile ID
66065602000000	FIRES	STRUCTURAL FIRES	Solid Fuel (Unspecified)	SUB-CATEGORY UNSPECIFIED	OG1492
66065802000000	FIRES	VEHICLE FIRES	Solid Fuel (Unspecified)	SUB-CATEGORY UNSPECIFIED	OG1496
67066002629874	MANAGED BURNING AND DISPOSAL	AGRICULTURAL BURNING - PRUNINGS	Agricultural Waste	RAISIN TRAYS	OG1494
67066202629866	MANAGED BURNING AND DISPOSAL	AGRICULTURAL BURNING - FIELD CROPS	Agricultural Waste	PAPER HOT CAPS	OG1494
67067002000000	MANAGED BURNING AND DISPOSAL	NON-AGRICULTURAL OPEN BURNING	Solid Fuel (Unspecified)	SUB-CATEGORY UNSPECIFIED	OG1493
67099502400000	MANAGED BURNING AND DISPOSAL	OTHER	Solid Waste (Unspecified)	SUB-CATEGORY UNSPECIFIED	OG1493
67099502409844	MANAGED BURNING AND DISPOSAL	OTHER	Solid Waste (Unspecified)	BROODER PAPER	OG1494

EIC/SCC	Category	Sub-Category 1	Sub-Category 2	Sub-Category 3	New OG Profile ID
67099502409854	MANAGED BURNING AND DISPOSAL	OTHER	Solid Waste (Unspecified)	FERTILIZER SACKS	OG1495
67099502409864	MANAGED BURNING AND DISPOSAL	OTHER	Solid Waste (Unspecified)	OTHER	OG1493
67099502409868	MANAGED BURNING AND DISPOSAL	OTHER	Solid Waste (Unspecified)	PESTICIDE/SEED SACKS	OG1495
93065702000000	WILDFIRES	WILDFIRE CAUSED STRUCTURAL FIRES	Solid Fuel (Unspecified)	SUB-CATEGORY UNSPECIFIED	OG1492
93065902000000	WILDFIRES	WILDFIRE CAUSED VEHICLE FIRES	Solid Fuel (Unspecified)	SUB-CATEGORY UNSPECIFIED	OG1496
50100201	SOLID WASTE DISPL	GOVERNMENT	OPEN BURNING DUMP	GENERAL	OG1493
50200202	SOLID WASTE DISPL	COMMERCL/INSTITNL	OPEN BURNING	REFUSE	OG1493
50300202	SOLID WASTE DISPL	INDUSTRIAL	OPEN BURNING	REFUSE	OG1493

EIC/SCC	Category	Sub-Category 1	Sub-Category 2	Sub-Category 3	New OG Profile ID
50300203	SOLID WASTE DISPL	INDUSTRIAL	OPEN BURNING	AUTO BODY COMPTS	OG1496

Table A2. List of new species to be added to CEIDARS database. For species lacking a CAS registry number, a PubChem ID is provided wherever available

SAROAD	Species	CAS/ PubChem ID	Formula	Mol Wt.	Type
51502	1,7,7-trimethyl-2-methylidenebicyclo[2.2.1]heptane	27538-47-2	C11H18	150.26	Compound
50761	1-chloro-1-propene	590-21-6	C3H5Cl	76.52	Compound
51361	1-chloro-3-ethynylbenzene	766-83-6	C8H5Cl	136.58	Compound
51501	1-phenoxy-2-propanone	621-87-4	C9H10O2	150.18	Compound
51111	2-acetyl-1-pyrroline	85213-22-5	C6H9NO	111.14	Compound
50871	2-chloroacrylonitrile	920-37-6	C3H2ClN	87.51	Compound
50881	chloropropiolaldehyde	59422039	C3HClO	88.49	Compound

SAROAD	Species	CAS/ PubChem ID	Formula	Mol Wt.	Type
51122	2-hydroxy-3-methyl-2-cyclopenten-1-one	80-71-7	C6H8O2	112.13	Compound
50512	2-propynenitrile	1070-71-9	C3HN	51.05	Compound
51243	3,3-dichloro-2-propenal	2648-51-3	C3H2Cl2O	124.95	Compound
50901	acryloyl chloride	814-68-6	C3H3ClO	90.51	Compound
51462	benzylideneacetone	1896-62-4	C10H10O	146.19	Compound
50851	chlorocyanoacetylene	2003-31-8	C3ClN	85.49	Compound
51642	cyclododecyne	1129-90-4	C12H20	164.29	Compound
51121	ethyl chlorate	21806692	C2H5ClO3	112.51	Compound
51621	hexamethylbenzene	87-85-4	C12H18	162.28	Compound
51491	hydroxymandelonitrile	23190910	C8H7NO2	149.15	Compound
51631	methcathinone	160977-88-8	C10H13NO	163.22	Compound
50883	methyl propionate	554-12-1	C4H8O2	88.11	Compound

SAROAD	Species	CAS/ PubChem ID	Formula	Mol Wt.	Type
50731	nitroethene	3638-64-0	C2H3NO2	73.05	Compound
51731	phenyl cyanate	1122-85-6	C7H5NO	119.12	Compound
51461	phenylpropiolic acid	637-44-5	C9H6O2	146.14	Compound
51641	phthalamide	88-96-0	C8H8N2O2	164.16	Compound
50701	propiolic acid	471-25-0	C3H2O2	70.05	Compound
51051	pyrazinecarbonitrile	19847-12-2	C5H3N3	105.1	Compound
50882	pyruvic acid	127-17-3	C3H4O3	88.06	Compound
51291	quinoline	91-22-5	C9H7N	129.16	Compound
51221	salicylaldehyde	90-02-8	C7H6O2	122.12	Compound
50991	succinimide	123-56-8	C4H5NO2	99.09	Compound
51341	terephthalaldehyde	623-27-8	C8H6O2	134.13	Compound
51721	terpenylic acid	26754-48-3	C8H12O4	172.18	Compound

SAROAD	Species	CAS/ PubChem ID	Formula	Mol Wt.	Type
50841	thiophene	110-02-1	C4H4S	84.14	Compound
51420	trichloropropyne	19010338	C3HCl3	143.39	Compound
99493	lumped structural fire organics				Mixture
99494	lumped refuse burning organics				Mixture
99495	lumped cellulosic burning organics				Mixture
99496	lumped polymer burning organics				Mixture

Table A3. Species-level TOG fractional contributions for the newly added speciation profiles (OG1492–OG1496).

SA-ROAD	Species	Formula	OG1492 (%)	OG1493 (%)	OG1494 (%)	OG1495 (%)	OG1496 (%)
43218	1,3-butadiene	C4H6	2.9228	3.7545	5.4933	3.9270	
51502	1,7,7-trimethyl-2-methylidenebi-cyclo[2.2.1]heptane	C11H18	0.0173	0.0098	0.0216	0.0000	
50761	1-chloro-1-propene	C3H5Cl	0.0012	0.0010	0.0018	0.0002	

SA-ROAD	Species	Formula	OG1492 (%)	OG1493 (%)	OG1494 (%)	OG1495 (%)	OG1496 (%)
51361	1-chloro-3-ethynylbenzene	C8H5Cl	0.0260	0.0259	0.0058	0.0398	
47048	1-hydroxy-2-propanone	C3H6O2	1.9784	1.1478	1.0641	0.0988	
51501	1-phenoxy-2-propanone	C9H10O2	0.1396	0.0665	0.0174	0.0017	
51111	2-acetyl-1-pyrroline	C6H9NO	0.0095	0.0082	0.0109	0.0056	
43552	2-butanone	C4H8O	0.2064	0.1406	0.0874	0.0007	
50871	2-chloroacrylonitrile	C3H2ClN	0.0140	0.0148	0.0290	0.0241	
51122	2-hydroxy-3-methyl-2-cyclopen-ten-1-one	C6H8O2	0.5267	0.2743	0.1521	0.0346	
50512	2-propynenitrile	C3HN	0.0158	0.0197	0.0136	0.0649	
51243	3,3-dichloro-2-propenal	C3H2Cl2O	0.0045	0.0059	0.0108	0.0040	
43503	acetaldehyde	C2H4O	2.0241	1.4815	1.7426	0.1502	4.2934
43404	acetic acid	C2H4O2	4.5799	2.9962	3.5725	0.3867	0.0000
47045	glycolaldehyde	C2H4O2	0.2411	0.1577	0.1880	0.0203	0.0000

SA-ROAD	Species	Formula	OG1492 (%)	OG1493 (%)	OG1494 (%)	OG1495 (%)	OG1496 (%)
99298	acetic anhydride	C4H6O3	0.4358	0.3353	0.4404	0.0817	
43551	acetone	C3H6O	0.6177	0.4982	0.3927	0.0243	
43702	acetonitrile	C2H3N	0.8271	0.8191	0.0242	2.3659	
43206	acetylene	C2H2	6.3410	8.1803	20.0145	14.3076	
43505	acrolein	C3H4O	1.6169	1.4219	1.6264	0.6350	3.1895
43704	acrylonitrile	C3H3N	1.7559	1.6018	0.5048	4.1531	
50901	acryloyl chloride	C3H3ClO	0.0758	0.0783	0.1233	0.0828	
45501	benzaldehyde	C7H6O	0.9637	0.9014	0.4856	1.2415	0.3603
45201	benzene	C6H6	6.6049	8.1260	3.8185	11.4249	1.7165
50313	benzofuran	C8H6O	0.3731	0.4422	0.1501	0.3605	
51031	benzonitrile	C7H5N	0.9369	1.0049	0.3785	2.1072	0.1080
98024	benzyl chloride	C7H7Cl	0.0245	0.0193	0.0186	0.0062	
51462	benzylideneacetone	C10H10O	0.1438	0.0737	0.0123	0.0060	

SA-ROAD	Species	Formula	OG1492 (%)	OG1493 (%)	OG1494 (%)	OG1495 (%)	OG1496 (%)
98050	c10 aromatics	C10H14	0.0790	0.0544	0.0963	0.0000	
43125	c10 olefins	C10H20	0.0075	0.0049	0.0137	0.0000	
43290	c8 alkenes	C8H16	0.0149	0.0085	0.0116	0.0000	
99336	c8 phenols	C8H10O	0.5473	0.2976	0.0779	0.0039	
98166	camphor	C10H16O	0.0334	0.0167	0.0215	0.0003	
98088	carvone	C10H14O	0.0582	0.0216	0.0115	0.0004	
45801	chlorobenzene	C6H5Cl	0.1095	0.1380	0.0766	0.2280	
50851	chlorocyanoacetylene	C3ClN	0.0030	0.0043	0.0082	0.0077	
50881	chloropropiolaldehyde	C3HClO	0.0039	0.0046	0.0093	0.0044	
51642	cyclododecyne	C12H20	0.0122	0.0059	0.0142	0.0000	
99248	dichlorobenzene (mixed isomers)	C6H4Cl2	0.0092	0.0111	0.0064	0.0131	
46751	dihydronaphthalene	C10H10	0.3120	0.2245	0.0655	0.0545	

SA-ROAD	Species	Formula	OG1492 (%)	OG1493 (%)	OG1494 (%)	OG1495 (%)	OG1496 (%)
99278	dimethyl sulfide	C2H6S	0.0006		0.0001	0.0003	
43202	ethane	C2H6	1.7207	1.0713			3.0345
43302	ethanol	C2H6O	0.0137	0.0118	0.0136	0.0097	
43203	ethene	C2H4	7.3295	11.2390	13.7475	9.8276	5.0634
51121	ethyl chlorate	C2H5ClO3	0.0200	0.0243	0.0045	0.0039	
45203	ethylbenzene	C8H10					0.1563
43502	formaldehyde	CH2O	1.6906	1.8343	3.7338	2.6691	7.4537
99902	furan	C4H4O	0.6070	0.5418	0.4632	0.1457	
99312	furfural	C5H4O2	1.0329	0.6929	0.8554	0.0627	
99026	furfuryl alcohol	C5H6O2	0.9088	0.5313	0.4722	0.0570	
43576	guaiacol	C7H8O2	1.0753	0.8020	0.4765	0.3548	
51621	hexamethylbenzene	C12H18	0.0283	0.0118	0.0166	0.0000	

SA-ROAD	Species	Formula	OG1492 (%)	OG1493 (%)	OG1494 (%)	OG1495 (%)	OG1496 (%)
43332	hydrogen cyanide	CHN	2.4462	3.9369	11.8033	8.4378	
51491	hydroxymandelonitrile	C8H7NO2	0.0343	0.0269	0.0052	0.0000	
43579	hydroxymethylfurfural	C6H6O3	0.1951	0.1491	0.1139	0.0417	
51240	hydroxyquinone	C6H4O3	0.0969	0.0583	0.0450	0.0073	
99173	isocyanic acid	CHNO	0.0191	0.0174	0.0269	0.0237	
43121	isomers of pentene	C5H10	0.1393	0.0914	0.1263	0.0000	
43152	isomers of undecyne	C11H20	0.0069	0.0039	0.0134	0.0000	
45102	isomers of xylene	C8H10	0.3860	0.3465	0.1627	0.0551	
43243	isoprene	C5H8	0.2610	0.2324	0.2636	0.0004	
43144	Lactic Acid	C3H6O3	0.0969	0.0718	0.1411	0.0218	
43201	methane	CH4	11.0966	15.9836	15.0688	10.7722	29.0989
51631	methcathinone	C10H13NO	0.0990	0.0216	0.0104	0.0003	

SA-ROAD	Species	Formula	OG1492 (%)	OG1493 (%)	OG1494 (%)	OG1495 (%)	OG1496 (%)
99180	methyl methacrylate	C5H8O2	0.5801	0.3907	0.3110	0.0000	
50883	methyl propionate	C4H8O2	0.3904	0.2380	0.2161	0.0100	
47041	methylbenzoic acids	C8H8O2	0.1957	0.1026	0.0512	0.0086	
43123	monoterpenes	C10H16	0.1802	0.1803	0.2003	0.0081	
98046	naphthalene	C10H8	2.1326	1.6470	0.0000	0.4805	
44250	nitroethane	C2H5NO2	0.0033	0.0020	0.0038	0.0003	
50731	nitroethene	C2H3NO2	0.2022	0.0947	0.0778	0.0323	
47023	nonanal	C9H18O	0.0370	0.0292	0.0970	0.0000	
45300	phenol	C6H6O	1.0082	1.0898	0.6282	0.7702	3.1937
51731	phenyl cyanate	C7H5NO	0.0248	0.0252	0.0313	0.0114	
51021	phenylacetylene	C8H6	1.7804	2.1583	0.0000	7.1744	0.0490
51461	phenylpropiolic acid	C9H6O2	0.1074	0.0534	0.0119	0.0021	

SA-ROAD	Species	Formula	OG1492 (%)	OG1493 (%)	OG1494 (%)	OG1495 (%)	OG1496 (%)
51641	phthalamide	C8H8N2O2	0.0331	0.0193	0.0022	0.0000	
98028	phthalic anhydride	C8H4O3	0.0704	0.0331	0.0123	0.0044	
43205	propene	C3H6	2.5488	2.3181			
50701	propiolic acid	C3H2O2	0.0540	0.0498	0.0499	0.0373	
51051	pyrazinecarbonitrile	C5H3N3	0.0063	0.0069	0.0040	0.0104	
43454	pyridine	C5H5N	0.1032	0.1131	0.0629	0.2956	0.2878
47050	pyrrole	C4H5N	0.5223	0.4379	0.0787	1.0023	
50882	pyruvic acid	C3H4O3	0.0755	0.0685	0.0961	0.0182	
51291	quinoline	C9H7N	0.2374	0.1419	0.0000	0.0809	
51221	salicylaldehyde	C7H6O2	0.8450	0.3474	0.2556	0.1857	
45220	styrene	C8H8	3.7895	3.3393	0.9545	6.4446	0.3405
50991	succinimide	C4H5NO2	0.0030	0.0023	0.0043	0.0028	

SA-ROAD	Species	Formula	OG1492 (%)	OG1493 (%)	OG1494 (%)	OG1495 (%)	OG1496 (%)
51341	terephthalaldehyde	C8H6O2	0.0719	0.0429	0.0126	0.0000	
45403	terephthalic acid	C8H6O4	0.0307	0.0174	0.0004	0.0000	
51721	terpenylic acid	C8H12O4	0.0805	0.0190	0.0073	0.0008	
50841	thiophene	C4H4S	0.2989	0.6700	0.0000	0.1282	
45202	toluene	C7H8	1.3067	1.4399	0.1451	2.2281	1.1030
51420	trichloropropyne	C3HCl3	0.0033	0.0059	0.0126	0.0030	
45107	trimethylbenzene	C9H12	0.0647	0.0515	0.0849	0.0000	
99999	unidentified	-	1.7130	1.3776	1.0316	0.8868	40.5515
43860	vinyl chloride	C2H3Cl	0.1572	0.0665	0.1094	0.0175	
99493	Lumped structural fire organics		17.4231				
99494	Lumped refuse burning organics			11.3213			
99495	Lumped cellulosic burning organics				7.0695		

SA-ROAD	Species	Formula	OG1492 (%)	OG1493 (%)	OG1494 (%)	OG1495 (%)	OG1496 (%)
99496	Lumped polymer burning organics					5.7968	
	Total		100.0000	100.0000	100.0000	100.0000	100.0000

Profile-specific lumped species

Newly added unresolved isomer-group entries were grouped into profile-specific lumped species for database implementation. Separate lumped species were used because the underlying grouped signals and their relative contributions differ by source profile. SAROAD 99493 was assigned to the OG1492 structural-fire lumped species, SAROAD 99494 was assigned to the OG1493 refuse/open-burning lumped species, SAROAD 99495 was assigned to the OG1494 cellulosic-burning lumped species, and SAROAD 99496 was assigned to the OG1495 synthetic-polymer-burning lumped species. No lumped species was created for OG1496 because the vehicle-fire profile did not include corresponding newly added unresolved isomer-group mass.

The lumped species preserve the total TOG mass assigned to these grouped signals while reducing the number of new database species requiring separate SAROAD records. The original internal composition of each lumped species is retained in the following appendix Table A4, including the contributing unresolved isomer groups, available chemical formulas. This documentation preserves traceability to the source measurements and allows the lumped species to be re-expanded in future updates if additional compound-level information becomes available.

Table A4. Internal composition of profile-specific lumped organic species used for unresolved isomer-group entries in the updated TOG profiles. Values represent the percent contribution of each original grouped species or isomer group to the corresponding lumped SAROAD species. SAROADs 99493, 99494, 99495, and 99496 correspond to the lumped species used for OG1492 structural fire, OG1493 refuse/open burning, OG1494 cellulosic material burning, and OG1495 synthetic-polymer burning, respectively.

Species	Formula	% of species 99493	% of species 99494	% of species 99495	% of species 99496
2-furanones	C4H4O2	2.7101	2.8081	5.5760	0.3571
3-dichlorocyclopentadienes	C5H4Cl2	0.0907	0.2084	0.4725	0.5589
benzoquinones	C6H4O2	1.0974	1.3576	2.1317	1.6406
benzothiophenes	C8H6S	2.0353	1.6792	0.0014	0.1535

Species	Formula	% of species 99493	% of species 99494	% of species 99495	% of species 99496
c2 substituted furans	C6H8O	4.0314	3.5872	3.6410	0.0207
c2 substituted pyrroles	C6H9N	0.0958	0.0521	0.1089	0.0000
chlorobenzaldehydes	C7H5ClO	0.0907	0.1308	0.0467	0.2363
chlorobenzamides	C7H6ClNO	0.1130	0.2084	0.1853	0.3727
chlorobenzoic acids	C7H5ClO2	0.0649	0.0787	0.0340	0.0345
chlorocatechols	C6H5ClO2	0.1848	0.1564	0.2121	0.0897
chlorocyclopentadiene isomers	C5H5Cl	0.2330	0.4487	0.7667	1.7752
chlorohexadieneones	C6H5ClO	1.2684	1.8533	2.3524	3.4589
chloropropyne isomers	C3H3Cl	0.0614	0.1272	0.3422	0.2414
chlorostyrenes	C8H7Cl	0.1114	0.1502	0.0651	0.2260
cyanoallene isomers (butadiene nitriles)	C4H3N	0.1045	0.1944	0.0848	1.3732
diacetylbenzenes	C10H10O2	0.7978	0.3127	0.4102	0.0812

Species	Formula	% of species 99493	% of species 99494	% of species 99495	% of species 99496
dichloroethylenes	C2H2Cl2	0.0207	0.0292	0.0665	0.0345
dihydroxybenzoic acids	C7H6O4	0.1763	0.1996	0.2023	0.1173
furan carbonitriles	C5H3NO	0.0087	0.0177	0.0807	0.1052
furanoic acids	C5H4O3	0.5665	0.5795	0.9292	0.1311
heptenes	C7H14	0.0172	0.0142	0.0609	0.0000
isomers of C10H11N	C10H11N	5.0950	1.3550	0.6677	0.1311
isomers of C10H12	C10H12	0.7089	0.7755	0.7554	0.0396
isomers of C10H20O	C10H20O	0.0700	0.0724	0.3918	0.0017
isomers of C10H8O	C10H8O	0.8592	0.8020	0.1443	0.2951
isomers of C11H12	C11H12	0.7856	0.5150	0.2475	0.0172
isomers of C11H14	C11H14	0.4196	0.3268	0.3296	0.0000
isomers of C12H10	C12H10	0.8937	0.3585	0.0340	0.0000
Isomers of C12H10O	C12H10O	0.0413	0.0344	0.0226	0.0104

Species	Formula	% of species 99493	% of species 99494	% of species 99495	% of species 99496
isomers of C12H16	C12H16	0.2088	0.1185	0.1258	0.0000
isomers of C2H6ClNO	C2H6ClNO	0.7961	0.8400	1.7243	0.0845
isomers of C3H4O2	C3H4O2	1.6449	1.6995	6.6340	0.0534
isomers of C4H4O3	C4H4O3	0.2480	0.2924	0.3947	0.1035
isomers of C4H6O	C4H6O	3.2869	4.0473	7.3951	1.9856
isomers of C4H6O2	C4H6O2	8.0065	7.6980	11.3978	1.2801
isomers of C4H7N	C4H7N	0.1234	0.0901	0.1117	0.0380
isomers of C5H10O	C5H10O	0.4196	0.3709	0.3663	0.0000
isomers of C5H11NO2	C5H11NO2	0.0839	0.1043	0.0424	0.2433
isomers of C5H4O	C5H4O	2.9271	3.4167	5.6142	3.3192
isomers of C5H6O	C5H6O	8.8528	9.0327	10.0063	1.5613
isomers of C5H7N	C5H7N	0.3782	0.3100	0.4937	0.2208
Isomers of C5H7NO	C5H7NO	0.1096	0.2173	0.3253	0.6573

Species	Formula	% of species 99493	% of species 99494	% of species 99495	% of species 99496
isomers of C5H7NO2	C5H7NO2	0.2400	0.1855	0.2744	0.1035
isomers of C5H8O	C5H8O	6.9350	4.5050	5.4304	0.5779
isomers of C5H8O3	C5H8O3	1.2994	1.2446	1.6409	0.1674
Isomers of C5HN	C5HN	0.0207	0.0406	0.0552	0.2174
isomers of C6H10O	C6H10O	0.4500	0.3675	0.8729	0.0000
isomers of C6H12O	C6H12O	0.2824	0.2225	0.6522	0.0000
isomers of C6H5N	C6H5N	0.4092	0.7526	0.8968	3.7970
isomers of C6H6O2	C6H6O2	4.5951	4.0067	3.8475	0.4969
isomers of C7H10O	C7H10O	0.8851	0.7093	0.6068	0.0000
isomers of C7H12O3	C7H12O3	0.3749	0.1969	0.1570	0.0207
isomers of C7H14O	C7H14O	0.4741	0.4602	1.8544	0.0017
isomers of C7H6O3	C7H6O3	0.5344	0.4345	0.7200	0.1018
isomers of C7H8O	C7H8O	2.7067	3.1411	1.8332	0.7676

Species	Formula	% of species 99493	% of species 99494	% of species 99495	% of species 99496
isomers of C8H16O	C8H16O	0.0805	0.0609	0.2164	0.0000
isomers of C8H7N	C8H7N	0.5579	0.7323	0.0000	3.0363
isomers of C8H8O	C8H8O	2.4910	3.2656	2.5023	5.6757
isomers of C9H10	C9H10	5.1254	6.3351	3.3298	9.1933
isomers of C9H12O	C9H12O	0.9108	0.5759	0.2207	0.0000
isomers of C9H14O	C9H14O	0.3524	0.2464	0.4130	0.0000
isomers of C9H8	C9H8	6.4965	10.7845	1.0411	26.9714
isomers of C9H9N	C9H9N	0.2634	0.1448	0.0890	0.1139
isopropoxyphenols	C9H12O2	1.4516	0.8162	0.3932	0.0000
methyl acetophenones	C9H10O	0.6336	0.5963	0.6267	0.1863
methylbenzofurans	C9H8O	1.3200	1.6359	0.6507	0.4934
methylnaphthalenes	C11H10	1.7821	1.0971	0.0410	0.0000
methylthiophenes	C5H6S	0.0992	0.4028	0.0000	0.1156

Species	Formula	% of species 99493	% of species 99494	% of species 99495	% of species 99496
monochlorobenzofurans	C8H5ClO	0.0649	0.0901	0.0480	0.0845
monochlorodioxin isomers	C4H3ClO2	0.0562	0.0980	0.2758	0.0794
monoterpene alcohols	C10H18O	0.0734	0.0663	0.2701	0.0000
naphthylamines	C10H9N	0.5171	0.2376	0.0636	0.1242
naphthylmethylamines	C11H11N	1.4021	0.2668	0.2716	0.0638
nitrophenylacetonitriles	C8H6N2O2	0.1390	0.1704	0.3084	0.0638
nitropropanes	C3H7NO2	2.0473	3.4308	2.1190	16.0973
nitropropenes	C3H5NO2	1.7356	1.7198	2.3835	3.6831
nonenals	C9H16O	0.0631	0.0609	0.2234	0.0000
pentanenitriles	C5H9N	0.0309	0.0177	0.0282	0.0017
phenylpropynal isomers	C9H6O	2.8468	3.6976	0.3111	4.5182
propynamide isomers	C3H3NO	0.1337	0.2023	0.1344	1.1352
thiophenecarbonitriles	C5H3NS	0.0992	0.1652	0.0000	0.2104

Species	Formula	% of species 99493	% of species 99494	% of species 99495	% of species 99496
undecenals	C11H20O	0.0430	0.0317	0.1330	0.0017
vinyl pyridines	C7H7N	0.1372	0.1131	0.0692	0.8488
Total		100.0000	100.0000	100.0000	100.0000