

Appendix B

Chemicals Analyzed in the *2000 Emergency Response Guidebook* Analysis

Table B.1 lists the chemicals analyzed in the *2000 Emergency Response Guidebook* (2000ERG) analysis in alphabetical order by U.S. Department of Transportation (DOT) name. Most of these materials are toxic by inhalation (TIH) materials; however, several are surrogates for generic table entries (e.g., 2-amino-2-methylpropanenitrile) or mildly toxic components of mixtures (e.g., benzene). For reference, the Chemical Abstract Services (CAS) number, boiling point, vapor pressure at 20°C, and toxicological data are provided. Additional chemical data used in the analysis include critical temperature, critical volume, melting point, heat of vaporization, liquid density, and specific heat of the liquid. For vapor pressure, heat of vaporization, liquid density, and specific heat of the liquid, temperature-dependent relationships were used.

Table B.1 Chemicals Analyzed in the 2000ERG Analysis^a

DOT Name	CAS No.	Molecular Weight	Boiling Point (°C)	Vapor Pressure at 20°C (kPa)	LC ₅₀ or LC _{LO} (ppm)	1-h Protective (ppm)	15-min Protective (ppm)	Basis
Acrolein	107-02-8	56.1	52.7	29.69	62	0.5	1	ERPG
Aldicarb	116-06-3	N/A	N/A	N/A	1	0.01	0.02	LC ₅₀
Allyl alcohol	107-18-6	58.1	97.1	2.491	1060	10	20	LC ₅₀
Allyl chloroformate	2937-50-0	120.5	112.9	6.194	5	0.05	0.2	LC ₅₀
Allyl isothiocyanate	57-06-7	99.2	150.7	0.516	28-S	1	2	ERPG-S
Allylamine	107-11-9	57.1	53.4	25.69	572	5	10	LC ₅₀
2-Amino-2-methylpropanenitrile	19355-69-2	84.1	159.5	0.099	112	1	2	LC ₅₀
Ammonia	7664-41-7	17	-33.5	854.5	7,338	200	400	ERPG
Arsenic trichloride	7784-34-1	181.2	130.1	1.113	56	0.5	1.0	LC _{LO}
Arsine	7784-42-1	77.9	-62.5	1475	30	0.5	0.6	ERPG
Benzene	71-43-2	78.1	80.1	9.983	26,458	150	300	ERPG
Bis-(2-chloroethyl) ethylamine	538-07-8	170.1	193.9	0.023	3.6	0.036	0.144	LC ₅₀
Bis-(2-chloroethyl) methylamine	51-75-2	156.1	174.9	0.039	7.8	0.078	0.312	LC ₅₀
Bis-(2-chloroethyl) sulfide	505-60-2	159.1	216.9	0.010	2.3	0.023	0.092	LC ₅₀
Boron tribromide	10294-33-4	251.5	89.0	7.336	387-S	3	6	LC ₅₀ -S
Boron trichloride	10294-34-5	117.2	12.5	132.2	2541	25	50	LC ₅₀
Boron trifluoride	7637-07-2	67.8	-99.8	4264	387	3	6	ERPG
Bromine	7726-95-6	159.8	58.8	22.87	310	1	2	ERPG
Bromine chloride	13863-41-7	115.4	4.9	220.0	290	3	6	LC ₅₀ -S
Bromine pentafluoride	7789-30-2	174.9	40.9	42.88	299-S	1	2	ERPG-S
Bromine trifluoride	7787-71-5	136.9	125.9	0.774	299-S	1	2	ERPG-S
Bromoacetone	598-31-2	137	135.9	11.431	95	1	2	LC _{LO}
n-Butyl chloroformate	592-34-7	136.6	137.9	0.765	323-S	3	6	LC ₅₀
sec-Butyl chloroformate	17462-58-7	136.6	127.9-E	1.051-E	323	3	6	LC ₅₀ -S
n-Butylisocyanate	111-36-4	99.1	115.0-S	1.755-S	28	0.05	0.1	ERPG
tert-Butyl-isocyanate	1609-86-5	99.1	86.0	4.888-E	22	0.05	0.1	ERPG-S
tert-Butylarsine	117791-53-4	134	44.4-E	40.35-E	140	1.5	3	LC ₅₀

Continued

Table B.1 Chemicals Analyzed in the 2000ERG Analysis^a (Cont.)

DOT Name	CAS No.	Molecular Weight	Boiling Point (°C)	Vapor Pressure at 20°C (kPa)	LC ₅₀ or LC _{LO} (ppm)	1-h Protective (ppm)	15-min Protective (ppm)	Basis
Carbon monoxide	630-08-0	28	-191.5	2792	4590	350	500	ERPG
Carbon tetrachloride	56-23-5	153.8	76.7	12.138	19,000	100	200	ERPG
Carbonyl fluoride	353-50-4	66	-84.6	5211	360	3	6	LC ₅₀
Carbonyl sulfide	463-58-1	60.1	-50.2	1124	924	10	20	LC ₅₀
Chlorine	7782-50-5	70.9	-34.1	679.7	293	3	6	ERPG
Chlorine pentafluoride	13637-63-3	130.4	-13.9	332.1	122	1	2	ERPG-S
Chlorine trifluoride	7790-91-2	92.4	11.8	148.0	299	1	2	ERPG
Chloroacetaldehyde	107-20-0	78.5	84.9	3.522	200	2	4	LC ₅₀
Chloroacetone	78-95-5	92.5	120.1	1.567	262	2	4	LC ₅₀
Chloroacetonitrile	107-14-2	75.5	126.0	1.087	500	5	10	LC ₅₀
Chloroacetyl chloride	79-04-9	112.9	106.0	2.522	660	1	2	ERPG
Chloromethyl methyl ether	107-30-2	80.5	59.5	21.14	441	3	6	LC ₅₀
p-Chlorophenyl isocyanate	104-12-1	153.6	199.0	0.069	18	0.15	0.3	LC ₅₀
Chloropicrin	76-06-2	164.4	111.9	3.190	28	0.2	0.4	ERPG
Chloropivaloyl chloride	4300-97-4	155	147.9	0.189-E	126	1	2	LC ₅₀
Chlorosulfonic acid	7790-94-5	116.5	153.9	0.309	929 mg/m ³	10 mg/m ³	20 mg/m ³	ERPG
Crotonaldehyde	4170-30-3	70.1	104.9	3.121	380	10	20	ERPG
Cyanogen	460-19-5	52	-21.2	489.7	350	3	6	LC ₅₀
Cyanogen chloride	506-77-4	61.5	12.9	135.0	80	0.4	1.0	ERPG
Cyclohexyl isocyanate	3173-53-3	125.2	169.0	0.094	15	0.05	0.1	ERPG-S
Cyclohexyl methylphosphonofluoridate	N/A	180.2	238.9	0.006	0.08	0.0008	0.0032	LC ₅₀

Continued



Table B.1 Chemicals Analyzed in the 2000ERG Analysis^a (Cont.)

DOT Name	CAS No.	Molecular Weight	Boiling Point (°C)	Vapor Pressure at 20°C (kPa)	LC ₅₀ or LC _{LO} (ppm)	1-h Protective (ppm)	15-min Protective (ppm)	Basis
Diamylamine	2050-92-2	157.3	203.0	0.013	126	1	2	LC _{LO}
Diborane	19287-45-7	27.7	-92.6	3438	80	1	2	ERPG
Dichlorosilane	4109-96-0	101	8.4	154.2	215	2	4	LC ₅₀
3,5-Dichloro-2,4,6-trifluoropyridine	1737-93-5	202	177.5-S	0.104-S	62	0.5	1	LC ₅₀
Diketene	674-82-8	84.1	126.1	1.064	612	5	10	ERPG
1,1-Dimethyl hydrazine	57-14-7	60.1	63.4	16.38	1410	15	30	LC ₅₀
1,2-Dimethyl hydrazine	540-73-8	60.1	87.1	7.230	680	7	15	LC ₅₀
Dimethyl sulfate	77-78-1	126.1	188.9	0.069	17	0.15	0.3	LC ₅₀
Diphosgene	503-38-8	197.8	127.9	0.553	50-S	0.1	0.2	ERPG-S
Ethyl chloroformate	541-41-3	108.5	92.9	2.121	145	1	2	LC ₅₀ -S
Ethylchlorothioformate	2812-73-9	124.6	131.9	0.685-E	138-S	1	2	LC ₅₀ -S
Ethylchlorothioformate	2941-64-2	124.6-S	131.9-S	0.685-S	138-S	1	2	LC ₅₀ -S
Ethyl dichloroarsine	598-14-1	174.9	155.9	0.281	36	0.3	0.6	LC ₅₀
Ethyl N,N-dimethylphosphoramidocyanidate	N/A	162.3	239.9-E	0.005-E	0.18	0.0018	0.0072	LC ₅₀
Ethyl isocyanate	109-90-0	71.1	61.6	24.50	28-S	0.05	0.1	ERPG-S
Ethyl phosphonothionic dichloride	993-43-1	162.9	176.9	0.026-E	62-S	0.5	1	LC ₅₀
Ethyl phosphonous dichloride	1498-40-4	130.9	113.0-E	4.762-E	62	0.5	1	LC _{LO}
Ethyl phosphorodichloridate	1498-51-7	162.9	166.9	0.040-E	43	0.3	0.6	LC ₅₀
Ethylacrolein	922-63-4	84.1	92.9	5.392-E	578	5	10	LC ₅₀
Ethylene chlorohydrin	107-07-3	80.5	128.7	0.699	74	0.5	1	LC ₅₀
Ethylene dibromide	106-93-4	187.9	131.4	1.357	691	5	10	LC ₅₀
Ethylene oxide	75-21-8	44.1	10.5	146.3	5840	50	100	ERPG
Ethylenimine	151-56-4	43.1	55.9	22.18	250	2	4	LC ₅₀
Fluorine	7782-41-4	38	-188.3	4160	185	5	15	ERPG
Germanium tetrachloride	10038-98-9	214.4	83.9	9.51	150	1	2	LC _{LO}
Germanium tetrahydride	7782-65-2	76.6	-88.2	3870	622	5	10	LC ₅₀

Continued

Table B.1 Chemicals Analyzed in the 2000ERG Analysis^a (Cont.)

DOT Name	CAS No.	Molecular Weight	Boiling Point (°C)	Vapor Pressure at 20°C (kPa)	LC ₅₀ or LC _{LO} (ppm)	1-h Protective (ppm)	15-min Protective (ppm)	Basis
Hexachlorocyclopentadiene	77-47-4	272.8	239.1	0.0052	3	0.03	0.06	LC ₅₀
Hexaethyltetraphosphate	757-58-4	506.2	-195.9	2644	24-E	0.5	1	LC ₅₀ -E
Hexafluoroacetone	684-16-2	166	-27.3	584.19	476	1	2	ERPG
Hydrogen bromide	10035-10-6	80.9	-66.8	2182	2860	20	40	ERPG-S
Hydrogen chloride	7647-01-0	36.5	-85.1	4206	3124	20	40	ERPG
Hydrogen cyanide	74-90-8	27	25.8	81.63	71	10	20	ERPG
Hydrogen fluoride	7664-39-3	20	19.6	102.7	1300	20	40	ERPG
Hydrogen iodide	10034-85-2	127.9	-35.6	691.0	2860	20	40	ERPG-S
Hydrogen selenide	7783-07-5	81	-42.1	911.1	4-6	0.05	0.1	LC ₅₀
Hydrogen sulfide	7783-06-4	34.1	-60.4	1781	712	30	60	ERPG
Iron pentacarbonyl	13463-40-6	195.9	102.8	3.142	57	0.5	1	LC ₅₀
Isobutyl chloroformate	543-27-1	136.6	128.1	0.751	299	3	6	LC ₅₀
Isobutyl isocyanate	1873-29-6	99.1	115.0	1.755	28-S	0.05	0.1	ERPG-S
Isopropyl chloroformate	108-23-6	122.6	104.9-S	4.698-S	299	3	6	LC ₅₀
Isopropyl isocyanate	1795-48-8	85.1	82.9	7.372	28-S	0.05	0.1	ERPG-S
Isopropyl methylphosphonofluoridate	107-44-8	140.1	157.9	0.283	0.1	0.001	0.004	LC ₅₀
Methacrylonitrile	126-98-7	67.1	90.4	7.541	656	5	10	LC ₅₀
Methanesulfonyl monochloride	124-63-0	114.6	162.4	0.190	5-S	0.05	0.01	LC ₅₀ -S
Methoxymethyl isocyanate	6427-21-0	87.1	165.7-E	0.250-E	28-S	0.05	0.1	ERPG-S
Methyl bromide	74-83-9	94.9	3.6	184.3	1007	50	100	ERPG
Methyl chloride	74-87-3	50.5	-24.3	495.4	11,040	400	1500	ERPG
Methyl chloroformate	79-22-1	94.5	70.9	11.20	88	1	2	LC ₅₀
Methyl hydrazine	60-34-4	46.1	87.6	4.997	148	1	2	LC ₅₀
Methyl iodide	74-88-4	141.9	42.5	44.33	1600	50	100	ERPG
Methyl isocyanate	624-83-9	57.1	38.9	50.18	41	0.5	1	ERPG
Methyl isothiocyanate	556-61-6	73.1	118.9	3.205	635	5	10	LC ₅₀
Methyl mercaptan	74-93-1	48.1	6.0	169.8	1340	25	50	ERPG

Continued



Table B.1 Chemicals Analyzed in the 2000ERG Analysis^a (Cont.)

DOT Name	CAS No.	Molecular Weight	Boiling Point (°C)	Vapor Pressure at 20°C (kPa)	LC ₅₀ or LC _{LO} (ppm)	1-h Protective (ppm)	15-min Protective (ppm)	Basis
Methyl phosphonic dichloride	676-97-1	132.9	162.9-E	0.040-E	52	0.5	1.0	LC ₅₀
Methyl phosphonous dichloride	676-83-5	116.9	81.9-E	11.89-E	52-S	0.5	1.0	LC ₅₀ -S
Methyl silicate	681-84-5	152.2	120.9	1.613	300	3	6	LC _{LO}
Methyl vinyl ketone	78-94-4	70.1	81.5	9.274	5	0.05	0.1	LC ₅₀
Methylamine	74-89-5	31.1	-6.3	295.7	5000	100	200	ERPG
Methylchlorosilane	993-00-0	80.6	8.8	149.6	1547-S	3	6	ERPG-S
Methyldichloroarsine	593-89-5	160.9	135.9	1.034	68	0.5	1	LC ₅₀
Nickel carbonyl	13463-39-3	170.8	42.5	43.50	18	0.15	0.3	LC ₅₀
Nitric acid	7697-37-2	63	83.0	6.401	67	1.3	2.6	LC ₅₀
Nitric oxide	10102-43-9	30	-151.8	5093	1708	15	30	LC ₅₀
Nitrogen dioxide	10102-44-0	46	21.0	96.04	115	10	20	EEL
Nitrogen fluoride oxide	13847-65-9	87.1	-129.1-E	3979-E	48	0.5	1.0	LC ₅₀
Nitrogen trioxide	10544-73-7	76	2.0	218.3	115-S	10	20	EEL
Nitrosyl chloride	2696-92-6	65.5	-5.3	270.4	293-S	3	6	ERPG-S
tert-Octyl mercaptan	141-59-3	146.3	155.9	0.488	102	1	2	LC ₅₀
O-Ethyl S-(2-diisopropylaminoethyl) methylphosphonothiolate	50782-69-9	267.4	297.9	.00005	0.023	0.00023	0.0009	LC ₅₀
Oxygen difluoride	7783-41-7	54	-145.0	2789	2.6	0.03	0.06	LC ₅₀
Parathion	56-38-2	291.3	-195.9	2644	14	0.15	0.3	LC ₅₀
Pentaborane	19624-22-7	63.2	58.4	22.70-E	10	0.1	0.2	LC ₅₀
Perchloromethyl mercaptan	594-42-3	185.9	148.0	0.642	69	0.5	1.0	LC ₅₀
Perchloryl fluoride	7616-94-6	102.4	-46.7	1060	770	5	10	LC ₅₀
Phenyl isocyanate	103-71-9	119.1	165.7	0.250	16	0.05	0.1	ERPG-S
Phenyl mercaptan	108-98-5	110.2	169.2	0.142	66	0.5	1.0	LC ₅₀
Phosgene	75-44-5	98.9	7.6	159.3	100	0.2	0.4	ERPG
Phosphine	7803-51-2	34	-87.8	3517	22	2.5	5	ERPG
Phosphorous oxychloride	10025-87-3	153.3	105.5	3.273	96	1	2	LC ₅₀
Phosphorous pentafluoride	7647-19-0	126	-84.6	19990-E	260	2	4	LC ₅₀ -S

Continued



Table B.1 Chemicals Analyzed in the 2000ERG Analysis^a (Cont.)

DOT Name	CAS No.	Molecular Weight	Boiling Point (°C)	Vapor Pressure at 20°C (kPa)	LC ₅₀ or LC _{LO} (ppm)	1-h Protective (ppm)	15-min Protective (ppm)	Basis
Phosphorous trichloride	7719-12-2	137.3	76.1	12.82	208	2	4	LC ₅₀
Phosphorous trifluoride	7783-55-3	88	-101.3	6902	433	3	6	LC ₅₀
Pinacolyl methylphosphonofluoridate	96-64-0	182.2	197.9	0.037	0.08	0.0008	0.0032	LC ₅₀
n-Propyl chloroformate	109-61-5	122.6	104.9	4.698	319	3	2	LC ₅₀
n-Propyl isocyanate	110-78-1	85.1	82.9	5.274	44	0.05	0.1	ERPG-S
Selenium hexafluoride	7783-79-1	193	-34.7	2854	50	0.5	1	LC ₅₀
Silicon tetrafluoride	7783-61-1	104.1	-95.2	3205	922	10	20	LC ₅₀
Stibine	7803-52-3	124.8	-18.5	286.1-E	20	0.5	1	ERPG
Sulfur chloride pentafluoride	13780-57-9	162.5	-21.2	442.0-S	100	1	2	LC _{LO}
Sulfur dioxide	7446-09-5	64.1	-10.1	336.5	2520	0.2	0.4	ERPG
Sulfur monochloride	10025-67-9	135	137.9	0.944	150*	1	2	LC ₅₀
Sulfur tetrafluoride	7783-60-0	108.1	-40.4	1785	40	0.4	0.8	LC ₅₀
Sulfur trioxide	7446-11-9	80.1	44.8	25.73	106 mg/m ³	10 mg/m ³	20 mg/m ³	ERPG
Sulfuryl chloride	7791-25-5	135	69.4	14.811	3020-S	30	60	LC ₅₀ -S
Sulfuryl fluoride	2699-79-8	102.1	-55.4	1964	3020	30	60	LC ₅₀
Tellurium hexafluoride	7783-80-4	241.6	-38.2	709.6	20	0.2	0.4	LC _{LO}
Tetraethyl dithiopyrophosphate	3689-24-5	322.3	-195.9	2644	1.5	0.015	0.02	LC ₅₀
Tetraethyl pyrophosphate	107-49-3	290.1	-195.9	2644	1.5-S	0.015	0.02	LC ₅₀ -S
Tetrafluorohydrazine	10036-47-2	104	-74.3	2515	950	10	20	LC ₅₀
Tetramethyl tin	594-27-4	178.8	77.9	17.92-E	58	0.6	1.2	LC _{LO}
Tetranitromethane	509-14-8	196	125.8	1.121	36	0.3	0.6	LC ₅₀
Thionyl chloride	7719-09-7	119	75.7	12.77	500	5	10	LC ₅₀
Thiophosgene	463-71-8	115	72.9	15.04	25-S	0.2	0.4	ERPG-S
Titanium tetrachloride	7550-45-0	189.7	135.9	1.253	1300 mg/m ³	20 mg/m ³	40 mg/m ³	ERPG
Trichloroacetyl chloride	76-02-8	181.8	118.0	2.189	128	1	2	ERPG-S
Trifluoroacetyl chloride	354-32-5	132.5	-17.9	356.2-S	208	1	2	ERPG-S

Continued





Table B.1 Chemicals Analyzed in the 2000ERG Analysis^a (Cont.)

DOT Name	CAS No.	Molecular Weight	Boiling Point (°C)	Vapor Pressure at 20°C (kPa)	LC ₅₀ or LC _{LO} (ppm)	1-h Protective (ppm)	15-min Protective (ppm)	Basis
Trifluorochloroethylene	79-38-9	116.5	-27.9	531.4	8568	100	200	ERPG
Trimethoxy silane	2487-90-3	122.3	80.9	20.40-E	84	2	4	ERPG
Trimethylacetyl chloride	3282-30-2	120.6	106.9	2.866	250	5	10	LC ₅₀
Tris-(2-chloroethyl) amine	817-09-4	204.5	255.9	0.00094	3	0.03	.12	LC ₅₀
Tungsten hexafluoride	7783-82-6	297.8	17.4	111.8	207	2	4	LC ₅₀

^a The abbreviations used in this table are defined as follows:

ERPG = Emergency Response Planning Guideline established by the American Industrial Hygiene Association (AIHA).

EEL = Emergency Exposure Level published in the *AIHA Journal*.

LC₅₀ = median lethal concentration in animals exposed via inhalation.

LC_{LO} = lowest lethal concentration reported in an animal study.

LC₅₀-E = LC₅₀ estimated from oral toxicity data.

E = estimated value.

S = data are for a structurally similar chemical.

N/A = not applicable.