

THE **SADTLER**

**STANDARD
SPECTRA**





SADTLER RESEARCH LABORATORIES, INC.

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TOXIC CHEMICALS

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TOXIC CHEMICALS

This collection contains 300 infrared spectrograms of a variety of substances which are considered to be hazardous to health. Some types of toxicity represented are irritants, narcotics, carcinogenics, etc., and for these substances Threshold Limit Values have been established by the American Conference of Governmental Industrial Hygienists (A.C.G.I.H.). The reference texts used for selection of compounds were the Handbook of Analytical Toxicology, 1969 published by The Chemical Rubber Company and the Toxic Substances List, 1972 Edition, published by the United States Department of Health, Education and Welfare.

The spectrograms used in this collection have been selected from various specific publications previously issued by Sadtler but now included in this single volume, infrared grating spectra have been used whenever possible and prism spectra only included when the corresponding grating spectrum was not available. Grating spectra are determined in the 4000 cm^{-1} to 250 cm^{-1} wavenumber region and are presented on a transmittance vs. linear frequency format, prism spectra are determined in the 2μ to 15μ wavelength region and are presented on a transmittance vs. linear wavelength format.

Each spectrogram is labelled with the name of the substance, molecular formula, molecular weight and original source of the substance. The method of sample preparation is also shown on each spectrogram, the preparation most frequently used is KBr Wafer or Capillary film except for the inorganic materials which were prepared as mineral oil mulls and the absorption due to the mineral oil indicated on the chart with asterisks, (*).

The indexes included with the collection show the spectrum number in the column headed TOXIC and the column headed PRISM shows the spectrum number for compounds previously published in the Sadtler Standard Prism Spectra Collection. There are four separate indexes: the numerical listing according to toxic spectrum number, the alphabetical listing according to chemical name, the molecular formula listing by ascending number of carbon atoms and the chemical classes listing according to functional groups.

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ETHINE	3961	6
ETHYNE	3961	6
ETHINE	3961	6
ACETYLENE	3961	6
ETHYNE	3961	6
10-AZANTHRACENE	1153	7
ACRIDINE	1153	7
PROPENAL /LIQUID/	6646	8
ACROLEIN /LIQUID/	6646	8
ACRYLALDEHYDE /LIQUID/	6646	8
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ACRYLONITRILE	386	10
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ACETIC ACID, SEC-BUTYL ESTER	5250	56
ACETIC ACID, TERT-BUTYL ESTER	18668	57
ACETIC ACID, 2-ETHOXYETHYL ESTER	5284	140
ACETIC ACID, ETHYL ESTER	4	141
ACETIC ACID, ISOBUTYL ESTER	164	165
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ACETONE	233	4
ACETONITRILE	269	5
ACETYLENE	3961	6
ACRIDINE	1153	7
ACROLEIN /LIQUID/	6646	8
ACRYLALDEHYDE /LIQUID/	6646	8
ACRYLAMIDE	2998	9
ACRYLIC ACID, ETHYL ESTER	1310	142
ACRYLIC ACID, METHYL ESTER	1117	184
ACRYLONITRILE	386	10
ALLYL ALCOHOL	284	11
ALLYL CHLORIDE	275	84
AMMONIA	93	15
AMMONIUM FLUORIDE		16
AMMONIUM SULFANATE		17
ANILINE	3695	18
ANILINE, P-AMINO-,	4111	237
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BENZENE, O-DICHLORO-,	1003	103
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BENZENE, P-DIHYDROXY-,	153	162
BENZENE, H-DINITRO-,	81	128
BENZENE, O-DINITRO-,	12397	129
BENZENE, P-DINITRO-,	3657	130
BENZENE, M-DIPHENYL-,	4542	257
BENZENE, O-DIPHENYL-,	4543	258
BENZENE, P-DIPHENYL-,	8568	259
BENZENE, ETHYL-,	246	144
BENZENE, ISOPROPYL-,	242	94
BENZENE, METHYL-,	419	271
BENZENE, NITRO-,	12	215
BENZENE, TETRAHYDRO-,	196	98
BENZENE, VINYL-,	241	255

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BENZIDINE	6632	39
BENZOL/F/	579	38
P-BENZOQUINONE	751	40
BENZOYL PEROXIDE	332	41
BENZYL CHLORIDE	8	85
BENZYL MEFCAPTAN	6615	272
BERYLLIUM HYDROXIDE		42
BERYLLIUM OXIDE		43
BICYCLO/2.2.1/HEPTAN-2-ONE, 1,7,7- TRIMETHYL-,	244	69
BIPHENYL	783	44
BIPHENYL, 4,4PP-DIAMINO-,	6632	39
BIVINYL	893	51
BORON OXIDE		46
BROMOPORM	10	276
1,3-BUTADIENE	893	51
BUTANAL	333	63
1-BUTANETHIOL	6613	52
1-BUTANOL	75	58
2-BUTANOL	5278	59
2-BUTANONE	297	53
2-BUTENAL	1457	93
BUTYL ALCOHOL	75	58
BUTYL ALCOHOL, ACETATE	1041	55
BUTYL ALCOHOL, TERP-,		60
BUTYLAMINE	6648	61
BUTYL PHOSPHATE	138	277
BUTYRALDEHYDE	333	63
CADMIUM FLUORIDE		64
CALCIUM ARSENATE		65
CALCIUM CHROMATE /VI/		66
CALCIUM HYDROXIDE		67
CALCIUM OXIDE		68
2-CAMPHANONE	244	69
CAMPHOR	244	69
CARBOLIC ACID	843	236
CARBON DIOXIDE	1924	70
CARBON DISULFIDE	2223	71
CARBONIC ACID, DIETHYL ESTER	8024	116
CARBON MONOXIDE	1142	72
CARBON TETRACHLORIDE	2210	73
CELLOSOLVE, BUTYL-,	2292	54
CHLOREX	13381	45
CHLOROFORM	2224	79
CHROMIC /VI/ ACID		87
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CHROMIUM /III/ OXIDE		88
CHRYSENE	1188	92
CINNAMENE	241	255
M-CRESOL	2338	89
O-CRESOL	844	90
O-CRESOL, 4,6-DINITRO-,	287	131
P-CRESOL	33	91
CROTONALDEHYDE	1457	93
CUMENE	242	94
2,5-CYCLOHEXADIENE-1,4-DIONE	751	40
CYCLOHEXANE	180	95
CYCLOHEXANE, METHYL-,	194	187
CYCLOHEXANOL	41	96
CYCLOHEXANOL, 2-METHYL-,	7395	188
CYCLOHEXANONE	166	97
CYCLOHEXANONE, 2-METHYL-,	8401	189
CYCLOHEXENE	196	98
2-CYCLOHEXEN-1-ONE, 3,5,5-TRIMETHYL-,	122	287
DECABORANE S	11849	99
DIETHYLAMINE /LIQUID/	3194	114
DIETHYLAMINE, 2,2PP-DIAMINO-,	5318	117
DIETHYLENETRIAMINE	5318	117
DIISOPROPYLAMINE	1059	118
DIMETHYLAMINE	1140	121
DIMETHYLAMINE, N-NITROSO-,	20605	219
D-DIOXANE	40	136
D-DIOXIN, TETRAHYDRO-,	40	136
DN 2	287	131
DNC	287	131
DNOC	287	131
DN	175	133
EPICHLOROHYDRIN	129	75
ETHANE, BROMO-,	4632	48

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NAME	PRISM	TOXIC
ETHANE, CHLORO-	533	76
ETHANE, 1,2-DIBROMO-	996	101
ETHANE, 1,1-DICHLORO-	3205	107
ETHANE, 1,2-DICHLORO-	35	108
ETHANE, 1,1-DICHLORO-1-NITRO-	1263	112
ETHANE, 1,2-DIFLUORO-1,1,2,2-TETRA- CHLORO-	6524	262
ETHANE, HEXACHLORO-	4546	158
ETHANE, 1,1,2,2-TETABROMO-	1465	260
ETHANE, 1,1,2,2-TETRACHLORO-	182	261
ETHANE, 1,1,1-TRICHLORO-	19461	278
ETHANE, 1,1,2-TRICHLORO-	9721	279
ETHANE, 1,1,2-TRICHLORO-1,2,2- TRIFLUORO-	23717	285
ETHANETHIOL	6306	138
ETHANOL	188	143
ETHANOL, 2-AMINO-	123	13
ETHANOL, 2-BUTOXY-	2292	54
ETHANOL, 2-CHLORO-	73	77
ETHANOL, 2-DIETHYLAMINO/-	143	115
ETHANOL, 2-ETHOXY-	5291	139
ETHANOL, 2-METHOXY-	254	182
ETHER, ALLYL GLYCIDYL	14914	12
ETHER, 2,3-EPOXYPROPYL PHENYL	450	137
ETHER, ETHYL /LIQUID/	1335	147
ETHER, ISOPROPYL	102	170
ETHER, PHENYL	4492	238
ETHER, BIS/2-CHLOROETHYL/-	13381	45
ETHINE	3961	6
ETHYL ACETATE	4	141
ETHYL ALCOHOL	188	143
ETHYL CARBONATE	8024	116
ETHYL CHLORIDE	533	76
ETHYLENE, CIS-1,2-DICHLORO-	3645	109
ETHYLENE, TETRACHLORO-	237	263
ETHYLENE, TRICHLORO-	185	280
ETHYLENEDIAMINE	5319	145
ETHYLENE DIBROMIDE	996	101
ETHYLENIMINE	11399	29
ETHYLENE OXIDE	1109	146
ETHYL ETHER /LIQUID/	1335	147
ETHYL MERCAPTAN	6306	138
ETHYNE	3961	6
FORMALDEHYDE	2538	150
FORMAMIDE, N,N-DIMETHYL-	156	123
FORMIC ACID	25	151
FORMIC ACID, ETHYL ESTER	2515	148
FORMIC ACID, METHYL ESTER	693	191
FREON 112	6524	262
FREON 113	23717	285
2-FURALDEHYDE	113	152
PURAN, TETRAHYDRO-	74	265
2,5-FURANDIONE	462	176
2-FURANMETHANOL	124	153
PURFURAL	113	152
PURPUROLE	113	152
PURPURYL ALCOHOL	124	153
GLYCIDOL	15765	154
HEPTANE	271	155
2-HEPTANONE	340	156
3-HEPTANONE	2034	157
3-HEPTANONE, 5-METHYL-	32062	192
4-HEPTANONE, 2,6-DIMETHYL-	99	124
HEXANE	678	159
HEXYLAMINE	433	160
HI INITIAL V M AND P NAPHTHA		204
HYDANTOIN, 1,3-DICHLORO-5,5- DIMETHYL-	14908	106
HYDPAZINE, HYDRATE	8673	161
HYDRAZINE, 1,1-DIMETHYL-	7647	125
HYDPAZINE, METHYL-	7650	193
HYDRAZINE, PHENYL-	3670	239
HYDROQUINOL	153	162
HYDROQUINONE	153	162
ISOBENZOPURAN, 1,3-DIHYDRO-1,3- DIOXO-	8656	240
1,3-ISOBENZOPURANDIONE	8656	240
ISOBUTYL ALCOHOL	16	166
ISOCYANIC ACID, METHYLENEDI-P- PHENYLENE ESTER	6532	190
ISOCYANIC ACID, METHYL ESTER	42701	194

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ISOPROPYL ETHER	102	170
KETONE, METHYL ETHYL,	297	53
KETONE, METHYL PROPYL,	2903	230
LEAD, TETRAETHYL-,	580	264
LEAD ARSENATE		171
LEAD CHROMATE /VI/		172
LITHIUM FLUORIDE		173
LITHIUM HYDRIDE		174
MAGNESIUM FLUORIDE		175
MALEIC ANHYDRIDE	462	176
MERCURY, BIS/ACETATO/-,	8411	177
MERCURY /I/ NITRATE	15078	179
MERCURY /II/ ACETATE	8411	177
MERCURY /II/ CYANIDE		178
METHACRYLIC ACID, METHYL ESTER	2226	195
METHANE, BROMO-,	1098	49
METHANE, BROMOCHLORO-,	204	47
METHANE, BROMOTRIFLUORO-,	2478	50
METHANE, CHLORO-,	842	80
METHANE, DIBROMODIFLUORO-,	6523	100
METHANE, DICHLORO-,	1011	111
METHANE, DICHLORODIFLUORO-,	30865	105
METHANE, DICHLOROFLUORO-,	1129	110
METHANE, FLUOROTRICHLORO-,	1113	281
METHANE, IODO-,	59	164
METHANE, NITRO-,	61	216
METHANE, TETRACHLORO-,	2210	73
METHANE, TETRAMITRO-,	2492	267
METHANE, TRIBROMO-,	10	276
METHANE, TRICHLORO-,	2224	79
METHANETHIOL	38238	180
METHANETHIOL, TRICHLORO-,		282
METHANOL /LIQUID/	1918	181
METHYLAL	9685	119
METHYL ALCOHOL /LIQUID/	1918	181
METHYL BROMIDE	1098	49
METHYLENE DICHLORIDE	1011	111
METHYL IODIDE	59	164
METHYL MERCAPTAN	38238	180
METHYL SULFATE	15332	127
MOLYBDENUM OXIDE		201
MORPHOLINE	100	202
MORPHOLINE, 4-ETHYL-,	11309	149
NAPHTHA, V.H. AND P 50 FLASH		203
NAPHTHALENE	865	206
NAPHTHALENE, 1-CHLORO-,	3659	81
NAPHTHALENE, OCTACHLORO-,		223
2-NAPHTHYLAMINE K	9640	207
NICKEL CARBONYL /POLYMER/ F	12182	208
NICKEL CHLORIDE		209
NICKEL FLUORIDE		210
NICKEL /I/ SULFANATE		211
NICKEL SULFATE		212
NICOTINE	1355	213
OCTANE	5245	224
OXALIC ACID	2962	225
OXAZINE, 2H-1,4-, TETRAHYDRO-,	100	202
OXIRANE	1109	146
2-OXIRANEMETHANOL	15765	154
PENTANE	690	227
1-PENTANOL	52	233
2-PENTANOL	803	228
2-PENTANOL, 4-METHYL-,	66	196
3-PENTANOL	804	229
2-PENTANONE	2903	230
2-PENTANONE, 4-HYDROXY-4-METHYL-,	356	163
2-PENTANONE, 4-METHYL-,	44	197
PENTYL ALCOHOL	52	233
PETROLEUM ETHER		234
PHENANTHRENE	810	235
PHENETHYLENE	241	255
PHENOL	843	236
PHENOL, 2,4-DINITRO-,	253	132
PHENOL, PENTACHLORO-,	279	226
PHENOL, 2,4,6-TRINITRO-,	3891	241
P-PHENYLENEDIAMINE	4111	237
PHENYL ETHER	4492	238
PHENYL PHOSPHATE	9066	289

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PHTHALIC ACID, DIISOCTYL ESTER	673	135
PHTHALIC ACID, DIMETHYL ESTER	1265	126
PHTHALIC ANHYDRIDE	8656	240
PICRIC ACID	3891	241
POTASSIUM CHROMATE /VI/		242
POTASSIUM FLUORIDE		243
PROPANE	6404	244
PROPANE, 1-ALLYLOXY-2,3-EPOXY-	14914	12
PROPANE, 1-CHLORO-2,3-EPOXY-	129	75
PROPANE, 1-CHLORO-1-NITRO-	943	83
PROPANE, 1,2-DICHLORO-	3208	113
PROPANE, 1,2-EPOXY-	2211	247
PROPANE, 1,2-EPOXY-3-PHENOXY-	450	137
PROPANE, 1-NITRO-	43	217
PROPANE, 2-NITRO-	1	218
PROPANE, 1,2,3-TRICHLORO-	4653	284
1-PROPANOL		64
1-PROPANOL, 2,3-EPOXY-	15765	154
2-PROPANOL	189	168
2-PROPANOL, 2-METHYL-	2	60
2-PROPANONE	233	4
PROPENAL /LIQUID/	6646	8
PROPENE, 3-CHLORO-	275	84
2-PROPEN-1-OL	284	11
PROPYL ALCOHOL	64	246
PROPYLENE OXIDE	2211	247
PROPYL NITRATE	42332	248
PYRIDINE	15	249
PYRIDINE, 2-AMINO-	1789	14
PYRROLIDINE, 1-METHYL-2-/3-PYRIDYL-/-	1355	213
QUINOL	153	162
P-QUINONE	751	40
SELENIUM DIOXIDE		250
SILVER NITRATE		251
SILVER OXIDE		252
SODIUM CHROMATE /VI/		253
SPIRITS	188	143
STYRENE	241	255
STYRENE, METHYL-		199
STYRENE, A-METHYL-	195	198
STYROL	241	255
SUCCINONITRILE, TETRAMETHYL-, S	11883	266
SULFUR DIOXIDE	841	256
TEL	580	264
M-TERPHENYL	4542	257
O-TERPHENYL	4543	258
P-TERPHENYL	8568	259
TETRYL	21134	200
THORIUM NITRATE, TETRAHYDRATE		268
THULIUM CHLORIDE		269
TITANIUM /IV/ OXIDE		270
A-TNT	21886	288
TOLUENE	419	271
TOLUENE, P-TEFT-BUTYL-	8311	62
TOLUENE, A-CHLORO-	8	85
TOLUENE, 2,4-DINITRO-	175	133
TOLUENE, 2,6-DINITRO-	17378	134
TOLUENE, M-NITRO-	183	220
TOLUENE, O-NITRO-	4692	221
TOLUENE, P-NITRO-	4693	222
TOLUENE, 2,4,6-TRINITRO-	21886	288
A-TOLUENETHIOL	6615	272
O-TOLUIDINE	1543	273
O-TOLYL PHOSPHATE	22	274
TREMOLITE	1750	275
TRIETHYLAMINE	227	286
TRITOL	21886	288
TROTYL OIL	21886	288
TURPENTINE, GUM		290
VANADIUM OXIDE		291
V M AND P NAPHTHA		205
VINYL CHLORIDE	1119	78
M-XYLENE	1045	293
O-XYLENE	11	294
P-XYLENE	2276	295
3,5-XYLIDINE	34116	296
YTTORIUM NITRATE		292
ZINC CYANIDE		297
ZINC OXIDE		298

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NAME	C	H	Br	Cl	F	I	N	O	P	S	SI	M	PRISM	TOXIC
METHANE, BROMOTRIFLUORO-	1			1	3								2478	50
METHANE, DIBROMODIFLUORO-	1		2	2									6523	100
METHANE, DICHLORODIFLUORO-	1		2	2									30865	105
METHANE, FLUOROTRICHORO-	1			3	1								1113	281
CARBON TETRACHLORIDE	1												2210	73
METHANE, TETRACHLORO-	1			4									2210	73
METHANE, TETRAMITRO-	1						4		8				2492	267
CARBON MONOXIDE	1								1				1142	72
CARBON DIOXIDE	1								2				1924	70
BARIUM CARBONATE	1									3		BA		31
CARBON DISULFIDE	1										2		2223	71
BROMOPORN	1	1	3										10	276
METHANE, TRIBROMO-	1	1	3										10	276
METHANE, DICHLOROFLURO-	1	1		2	1								1129	110
CHLOROPORN	1	1		3									2224	79
METHANE, TRICHLORO-	1	1		3									2224	79
METHANETHIOL, TRICHLORO-	1	1		3						1				282
METHANE, BROMOCHLORO-	1	2	1	1									204	47
METHANE, DICHLORO-	1	2	2										1011	111
METHYLENE DICHLORIDE	1	2	2										1011	111
FORMALDEHYDE	1	2							1				2538	150
FORMIC ACID	1	2							2				25	151
METHANE, BROMO-	1	3	1										1098	49
METHYL BROMIDE	1	3	1										1098	49
METHANE, CHLORO-	1	3		1									842	80
METHANE, IODO-	1	3			1								59	164
METHYL IODIDE	1	3			1								59	164
METHANE, NITRO-	1	3					1		2				61	216
METHANOL /LIQUID/	1	4							1				1918	181
METHYL ALCOHOL /LIQUID/	1	4							1				1918	181
METHANETHIOL	1	4								1			38238	180
METHYL MERCAPTAN	1	4								1			38238	180
HYDRAZINE, METHYL-	1	6					2						7650	193
ETHANE, 1,1,2-TRICHLORO-1,2,2- TRIFLUORO-	2			3	3								23717	285
FREON 113	2			3	3								23717	285
ETHYLENE, TETRACHLORO-	2			4									237	263
ETHANE, 1,2-DIFLUORO-1,1,2,2-TETRA- CHLORO-	2			4	2								6524	262
FREON 112	2			4	2								6524	262
ETHANE, HEXACHLORO-	2			6									4546	158
MERCURY /II/ CYANIDE	2						2				HG			178
ZINC CYANIDE	2						2				ZN			297
BARIUM THIOCYANATE, HYDRATED	2						2			2	BA			37
NICKEL CARBONYL /POLYMER/ P	2							2			NI		12182	208
ETHYLENE, TRICHLORO-	2	1		3									185	280
ACETYLENE	2	2											3961	6
ETHINE	2	2											3961	6
ETHYNE	2	2											3961	6
ETHANE, 1,1,2,2-TETRABROMO-	2	2		4									1465	260
ETHYLENE, CIS-1,2-DICHLORO-	2	2		2									3645	109
ETHANE, 1,1,2,2-TETRACHLORO-	2	2		4									182	261
ACETIC ACID, FLURO-, SODIUM SALT	2	2		1				2			NA		17459	254
OXALIC ACID	2	2						4					2962	225
VINYL CHLORIDE	2	3		1									1119	78
ETHANE, 1,1-DICHLORO-1-NITRO-	2	3		2			1	2					1263	112
ETHANE, 1,1,1-TRICHLORO-	2	3		3									19461	278
ETHANE, 1,1,2-TRICHLORO-	2	3		3									9721	279
ACETONITRILE	2	3			1								269	5
ISOCYANIC ACID, METHYL ESTER	2	3			1		1						42701	194
ETHANE, 1,2-DIBROMO-	2	4	2										996	101
ETHYLENE DIBROMIDE	2	4	2										996	101
ETHANE, 1,1-DICHLORO-	2	4		2									3205	107
ETHANE, 1,2-DICHLORO-	2	4		2									35	108
ACETALDEHYDE GAS	2	4						1					5824	1
ETHYLENE OXIDE	2	4						1					1109	146
OXIRANE	2	4						1					1109	146
ACETIC ACID	2	4						2					76	2
FORMIC ACID, METHYL ESTER	2	4						2					693	191
ETHANE, BROMO-	2	5	1										4632	48
ETHANE, CHLORO-	2	5		1									533	76
ETHYL CHLORIDE	2	5		1									533	76
ETHANOL, 2-CHLORO-	2	5		1				1					73	77
AZIRIDINE	2	5					1						11399	29
ETHYLENIMINE	2	5					1						11399	29
DIETHYLAMINE, N-NITROSO-	2	6					2	1					20605	219
ETHANOL	2	6						1					188	143
ETHYL ALCOHOL	2	6						1					188	143