

SUPPLEMENTARY DATA

Table S1. Differences between the classification categories “NO” and “n.a.” for the classifications

	Source	Description	Consulted documentation	Reference
NO	NTP, NIOSH, IARC	Chemical not classified as carcinogen	Specific	15,17,20
n.a.	ECHA-CLP, EPA, ACGIH	Classification for chemicals is not available	Unspecific	11,12,14,16

IARC: International Agency for Research on Cancer; **NTP:** National Toxicology Program (United States); **NIOSH:** National Institute for Occupational Safety and Health (United States); **EPA:** Environmental Protection Agency (United States); **ACGIH:** American Conference of Governmental Industrial Hygienists (United States); **n.a.:** not available

PART 1: THE DATABASE

The database is an Excel file freely available at the following link: <https://www.dropbox.com/scl/fi/fccr7dp5snfe71e50jva3/CARCINOSYS-Database.xlsx?rlkey=fozuomf30mntbkhfjmn3z3dv&dl=0>

The database is composed by 4 sheets.

Sheet 1: Disclaimer

Sheet 2: Table with the comparison between the CoCs consulted and their conversion in the CLP-COC.

Sheet 3: Glossary and legend.

Sheet 4: The tool.

The tool is structured in 11 columns and 84 rows. Columns report the substance information, its classifications (reference CLP, IARC, EPA, ACGIH, NTP, IARC CoCs) and some note concerning annotations and links. There are 83 substances.

The Table S2 reports the columns information of the tool.

Table S2 . Columns information of the tool.

Column	Column name	Column information
A	ID	Identifier number
B	CAS	Chemical Abstract Service Registry Number
C	CLP NAME	Chemical name used in the CLP CoC
D	CLP classification	CLP chemical classification
E	IARC (converted in CLP-equivalent classification)	IARC chemical classification converted in CLP CoC
F	EPA (converted in CLP-equivalent classification)	EPA chemical classification converted in CLP CoC
G	ACGIH (converted in CLP-equivalent classification)	ACGIH chemical classification converted in CLP CoC
H	NTP (converted in CLP-equivalent classification)	NTP chemical classification converted in CLP CoC
I	NIOSH (converted in CLP-equivalent classification)	NIOSH chemical classification converted in CLP CoC
J	Note	Abbreviated notes
K	Added documentation	Links and other

PART 2: ORIGINAL CoCs.

Table S3. Original CLP, IARC, EPA, ACGIH, NTP and NIOSH classification.

CAS	CLP Name	CLP	IARC	EPA	ACGIH	NTP	NIOSH
70-25-7	1-methyl-3-nitro-1-nitrosoguanidine	1B	2A	na	na	Reasonably Anticipated To Be Human Carcinogens	NO
96-12-8	1,2-dibromo-3-chloropropane	1B	2B	na	na	Reasonably Anticipated To Be Human Carcinogens	C
1746-01-6	2,3,7,8-tetrachlorodibenzo[b,e][1,4]dioxin	NO	1	na	na	Known To Be Human Carcinogens	C
71-43-2	benzene	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
542-88-1	bis(chloromethyl) ether; oxybis(chloromethane)	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
12001-28-4; 132207-32-0; 12172-73-5; 77536-66-4; 77536-68-6; 77536-67-5; 12001-29-5	Asbestos [actinolite, amosite (grunerite), antofillite, crisotilo, crocidolite, tremolite]	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
75-01-4	vinyl chloride; chloroethylene	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
1336-36-3	polychlorobiphenyls; PCB	NO	1	Likely to be Carcinogenic to Humans	na	reasonably Anticipated To Be Human Carcinogens	NO
106-89-8	1-chloro-2,3-epoxypropane; epichlorhydrin	1B	2A	Likely to be Carcinogenic to Humans	A3	Reasonably Anticipated To Be Human Carcinogens	C
50-00-0	formaldehyde	1B	1	Likely to be Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
50-32-8	benzo[a]pyrene; benzo[def]chrysene	1B	1	Carcinogenic to Humans	A2	Reasonably Anticipated To Be Human Carcinogens	NO
75-21-8	ethylene oxide; oxirane	1B	1	Carcinogenic to Humans	A2	Known To Be Human Carcinogens	C

127-18-4	tetrachloroethylene	2	2A	Likely to be Carcinogenic to Humans	A3	Reasonably Anticipated To Be Human Carcinogens	C
1327-53-3	diarsenic trioxide; arsenic trioxide	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
1303-28-2	diarsenic pentaoxide; arsenic pentoxide; arsenic oxide	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
na	arsenic acid and its salts with the exception of those specified elsewhere in this Annex	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
107-06-2	1,2-dichloroethane; ethylene dichloride	1B	2B	Likely to be Carcinogenic to Humans	A4	Reasonably Anticipated To Be Human Carcinogens	C
101-14-4	2,2'-dichloro-4,4'-methylenedianiline; 4,4'-methylene bis(2-chloroaniline)	1B	1	na	A2	Reasonably Anticipated To Be Human Carcinogens	C
24613-89-6	dichromium tris(chromate); chromium III chromate; chromic chromate	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
7789-06-2	strontium chromate	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
11103-86-9	zinc chromates including zinc potassium chromate	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
98-87-3	α,α -dichlorotoluene; benzylidene chloride; benzal chloride	2	2A	na	na	na	NO
100-44-7	α -chlorotoluene; benzyl chloride	1B	2A	Likely to be Carcinogenic to Humans	A3	na	NO
98-88-4	benzoyl chloride	NO	2A	na	A4	na	NO
53-70-3	dibenz[a,h]anthracene	1B	2A	Likely to be Carcinogenic to Humans	na	Reasonably Anticipated To Be Human Carcinogens	NO
191-30-0	dibenzo[def,p]chrysene; dibenzo[a,l]pyrene	1B	2A	na	na	Reasonably Anticipated To Be Human Carcinogens	NO
27208-37-3	cyclopenta [c,d] pyrene	na	2A	na	na	na	NO
90640-80-5	anthracene oil; [A complex combination of polycyclic aromatic hydrocarbons obtained from coal tar having an approximate distillation range of 300 °C to 400 °C (572 °F to 752 °F). Composed	1B	3	D (non cancerogenic)	na	na	NO

	primarily of phenanthrene, anthracene and carbazole.]						
8001-58-9	creosote; [The distillate of coal tar produced by the high temperature carbonization of bituminous coal. It consists primarily of aromatic hydrocarbons, tar acids and tar bases.]	1B	2A	Likely to be Carcinogenic to Humans	na	na	C
12510-42-8	erionite	1A	1	na	na	Known To Be Human Carcinogens	NO
650-017-00-8	RCF-Refractory Ceramic Fibres	1B	2B	Likely to be Carcinogenic to Humans	A2	Reasonably Anticipated To Be Human Carcinogens	NO
65996-93-2	pitch, coal tar, high-temp.,; [The residue from the distillation of high temperature coal tar. A black solid with an approximate softening point from 30 °C to 180 °C (86 °F to 356 °F). Composed primarily of a complex mixture of three or more membered condensed ring aromatic hydrocarbons.]	1A	1	na	A1	na	C
96-18-4	1,2,3-trichloropropane	1B	2A	Likely to be carcinogenic to humans	na	Reasonably Anticipated To Be Human Carcinogens	C
121-14-2	2,4-dinitrotoluene [1] dinitrotoluene [2]	1B	2B	na	na	na	C
106-99-0	1,3-butadiene; buta-1,3-diene	1A	1	Carcinogenic to humans	A2	Known To Be Human Carcinogens	NO
106-97-8	butane (containing ≥ 0,1 % butadiene (203-450-8))	1A	NO	na	na	na	NO
75-28-5	isobutane (containing ≥ 0,1 % butadiene (203-450-8))	1A	NO	na	na	na	NO
101-77-9	4,4'-diaminodiphenylmethane; 4,4'-methylenedianiline	1B	2B	na	A3	Reasonably Anticipated To Be Human Carcinogens	NO
79-06-1	acrylamide; prop-2-enamide	1B	2A	Likely to be carcinogenic to humans	A2	Reasonably Anticipated To Be Human Carcinogens	C
593-60-2	bromoethylene	1B	2A	na	A2	Reasonably Anticipated To Be Human Carcinogens	C

119-90-4	3,3'-dimethoxybenzidine; o-dianisidine	1B	2B	na	na	Reasonably Anticipated To Be Human Carcinogens	C
2425-06-1	captafol (ISO); 1,2,3,6-tetrahydro-N-(1,1,2,2-tetrachloroethylthio)phthalimide	1B	2A	na	A3	Reasonably Anticipated To Be Human Carcinogens	C
77-78-1	dimethyl sulphate	1B	2A	Likely to be Carcinogenic to Humans	A3	Reasonably Anticipated To Be Human Carcinogens	C
79-44-7	dimethylcarbamoyl chloride	1B	2A	na	A2	Reasonably Anticipated To Be Human Carcinogens	C
75-02-5	fluoroethylene	1B	2A	na	A2	Reasonably Anticipated To Be Human Carcinogens	NO
556-52-5	2,3-epoxypropan-1-ol; glycidol; oxiranemethanol	1B	2A	na	A3	Reasonably Anticipated To Be Human Carcinogens	NO
96-09-3	styrene oxide; (epoxyethyl)benzene; phenyloxirane	1B	2A	na	A3	Reasonably Anticipated To Be Human Carcinogens	NO
79-01-6	trichloroethylene; trichloroethene	1B	1	Carcinogenic to humans	A2	Known To Be Human Carcinogens	C
126-72-7	tris(2,3-dibromopropyl) phosphate	1B	2A	na	na	Reasonably Anticipated To Be Human Carcinogens	NO
7758-97-6	lead chromate	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
1344-37-2	lead sulfochromate yellow; C.I. Pigment Yellow 34; [This substance is identified in the Colour Index by Colour Index Constitution Number, C.I. 77603.]	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
12656-85-8	lead chromate molybdate sulfate red; C.I. Pigment Red 104; [This substance is identified in the Colour Index by Colour Index Constitution Number, C.I. 77605.]	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
1333-82-0	chromium (VI) trioxide	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
na	acids generated from chromium trioxide and their oligomers	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
na	oligomers of chromic acid and dichromic acid	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
7738-94-5	chromic acid	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C

13530-68-2	dichromic acid	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
10588-01-9, 7789-12-0	sodium dichromate	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
7778-50-9	potassium dichromate	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
7789-09-5	ammonium dichromate	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
7789-00-6	potassium chromate	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
7775-11-3	sodium chromate	1B	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
234-329-8	potassium hydroxyoctaoxodizincatedichromate	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
49663-84-5	pentazinc chromate octahydroxide	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
95-53-4	o-toluidine; 2-aminotoluene	1B	1	na	A3	Known To Be Human Carcinogens	C
95-69-2	4-chloro-o-toluidine [1] 4-chloro-o-toluidine hydrochloride [2]	1B	2A	na	na	Reasonably Anticipated To Be Human Carcinogens	NO
92-87-5	benzidine; 1,1'-biphenyl-4,4'-diamine; 4,4'-diaminobiphenyl; biphenyl-4,4'-ylenediamine	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
91-59-8	2-naphthylamine	1A	1	na	A1	Known To Be Human Carcinogens	C
92-67-1	biphenyl-4-ylamine; xenylamine; 4-aminobiphenyl	1A	1	na	A1	Known To Be Human Carcinogens	C
12070-12-1	tungsten carbide	NO	2A	na	A2	Reasonably Anticipated To Be Human Carcinogens	NO
7440-48-4	cobalt	1B	2A	na	A3	Reasonably Anticipated To Be Human Carcinogens	NO
7440-38-2	arsenic	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
na	arsenic compounds, with the exception of those specified elsewhere in ANNEX VI CLP-ATP 18	na	1	Carcinogenic to Humans	A2	Known To Be Human Carcinogens	C

7440-41-7	beryllium	1B	1	Likely to be Carcinogenic to Humans	A1	Known To Be Human Carcinogens	C
na	beryllium compounds with the exception of aluminium beryllium silicates, and with those specified elsewhere in this Annex	1B	1	Likely to be Carcinogenic to Humans	A2	Known To Be Human Carcinogens	C
7440-43-9	cadmium (pyrophoric)	1B	1	Likely to be Carcinogenic to Humans	A2	Known To Be Human Carcinogens	NO
7440-43-9 [1] 1306-19-0 [2]	cadmium (non-pyrophoric) [1] cadmium oxide (non-pyrophoric) [2]	1B	1	Likely to be Carcinogenic to Humans	A2	Known To Be Human Carcinogens	NO
7440-02-0	nickel	2	2B	non cancer	A5	Reasonably Anticipated To Be Human Carcinogens	C
13463-39-3	tetracarbonylnickel; nickel tetracarbonyl	2	1	Likely to be Carcinogenic to Humans	A3	Known To Be Human Carcinogens	C
12035-72-2	nickel subsulfide	1A	1	Carcinogenic to Humans	A1	Known To Be Human Carcinogens	NO
na	wood dusts	na	1	na	A1-A2-A4	Known To Be Human Carcinogens	C
14808-60-7	quartz (SiO ₂)	1A	1	na	A2	Known To Be Human Carcinogens	C
na	soot	na	1	na	na	Known To Be Human Carcinogens	NO

CAS: Chemical Abstract Service Registry Number; **CLP:** Classification Labelling Packaging; **EPA:** Environmental Protection Agency (United States); **ACGIH:** American Conference of Governmental Industrial Hygienists (United States); **NTP:** National Toxicology Program (United States); **IARC:** International Agency for Research on Cancer; **NIOSH:** National Institute for Occupational Safety and Health (United States); C: carcinogen; NO: non carcinogen; Na: not available.

PART 3: CoCs CONVERTED in CLP CoC

Table S4. Conversion of IARC, EPA, ACGIH, NTP and NIOSH classification in the reference CLP CoC.

CAS	CLP name	CLP	IARC	EPA	ACGIH	NTP	NIOSH
70-25-7	1-methyl-3-nitro-1-nitrosoguanidine	1B	1B	na	na	1B/2	NO
96-12-8	1,2-dibromo-3-chloropropane	1B	1B/2	na	na	1B/2	C
1746-01-6	2,3,7,8-tetrachlorodibenzo[b,e][1,4]dioxin	na	1A	na	na	1A	C
71-43-2	benzene	1A	1A	1A	1A	1A	C
542-88-1	bis(chloromethyl) ether; oxybis(chloromethane)	1A	1A	1A	1A	1A	C
12001-28-4; 132207-32-0; 12172-73-5; 77536-66-4; 77536-68-6; 77536-67-5; 12001-29-5	Asbestos [actinolite, amosite (grunerite), antofillite, crisotilo, crocidolite, tremolite]	1A	1A	1A	1A	1A	C
75-01-4	vinyl chloride; chloroethylene	1A	1A	1A	1A	1A	C
1336-36-3	polychlorobiphenyls; PCB	na	1A	1B	na	1B/2	NO
106-89-8	1-chloro-2,3-epoxypropane; epichlorhydrin	1B	1B	1B	2	1B/2	C
50-00-0	formaldehyde	1B	1A	1B	1A	1A	C
50-32-8	benzo[a]pyrene; benzo[def]chrysene	1B	1A	1A	1B	1B/2	C
75-21-8	ethylene oxide; oxirane	1B	1A	1A	1B	1A	C
127-18-4	tetrachloroethylene	2	1B	1B	2	1B/2	C
1327-53-3	diarsenic trioxide; arsenic trioxide	1A	1A	1A	1A	1A	C
1303-28-2	diarsenic pentaoxide; arsenic pentoxide; arsenic oxide	1A	1A	1A	1A	1A	C
na	arsenic acid and its salts with the exception of those specified elsewhere in this Annex	1A	1A	1A	1A	1A	C
107-06-2	1,2-dichloroethane; ethylene dichloride	1B	1B/2	1B	NO	1B/2	C
101-14-4	2,2'-dichloro-4,4'- methylenedianiline; 4,4'-methylene bis(2-chloroaniline)	1B	1A	na	1B	1B/2	C
24613-89-6	dichromium tris(chromate); chromium III chromate; chromic chromate	1B	1A	1A	1A	1A	C
7789-06-2	strontium chromate	1B	1A	1A	1A	1A	C
11103-86-9	zinc chromates including zinc potassium chromate	1A	1A	1A	1A	1A	C
98-87-3	α,α -dichlorotoluene; benzylidene chloride; benzal chloride	2	1B	na	na	NO	NO
100-44-7	α -chlorotoluene; benzyl chloride	1B	1B	1B	2	NO	NO
98-88-4	benzoyl chloride	na	1B	na	NO	NO	NO
53-70-3	dibenz[a,h]anthracene	1B	1B	1B	na	1B/2	C

191-30-0	dibenzo[def,p]chrysene; dibenzo[a,l]pyrene	1B	1B	na	na	1B/2	C
27208-37-3	cyclopenta [c,d] pyrene	na	1B	na	na	1B	C
90640-80-5	anthracene oil; [A complex combination of polycyclic aromatic hydrocarbons obtained from coal tar having an approximate distillation range of 300 °C to 400 °C (572 °F to 752 °F). Composed primarily of phenanthrene, anthracene and carbazole.]	1B	NO	na	na	1B	C
8001-58-9	creosote; [The distillate of coal tar produced by the high temperature carbonization of bituminous coal. It consists primarily of aromatic hydrocarbons, tar acids and tar bases.]	1B	1B	1B	na	1B	C
12510-42-8	erionite	1A	1A	na	na	1A	NO
650-017-00-8	RCF-Refractory Ceramic Fibres	1B	2	1B	1B	1B/2	NO
65996-93-2	pitch, coal tar, high-temp.,; [The residue from the distillation of high temperature coal tar. A black solid with an approximate softening point from 30 °C to 180 °C (86 °F to 356 °F). Composed primarily of a complex mixture of three or more membered condensed ring aromatic hydrocarbons.]	1A	1A	na	1A	1A	C
96-18-4	1,2,3-trichloropropane	1B	1B	1B	na	1B/2	C
121-14-2	2,4-dinitrotoluene [1] dinitrotoluene [2]	1B	1B/2	na	na	NO	C
106-99-0	1,3-butadiene; buta-1,3-diene	1A	1A	1A	1B	1A	NO
106-97-8	butane (containing ≥ 0,1 % butadiene (203-450-8))	1A	NO	na	na	NO	NO
75-28-5	isobutane (containing ≥ 0,1 % butadiene (203-450-8))	1A	NO	na	na	NO	NO
101-77-9	4,4'-diaminodiphenylmethane; 4,4'-methylenedianiline	1B	1B/2	na	2	1B/2	NO
79-06-1	acrylamide; prop-2-enamide	1B	1B	1B	1B	1B/2	C
593-60-2	bromoethylene	1B	1B	na	1B	1B/2	C
119-90-4	3,3'-dimethoxybenzidine; o-dianisidine	1B	1B/2	na	na	1B/2	C
2425-06-1	captafol (ISO); 1,2,3,6-tetrahydro-N-(1,1,2,2-tetrachloroethylthio)phthalimide	1B	1B	na	2	1B/2	C
77-78-1	dimethyl sulphate	1B	1B	1B	2	1B/2	C
79-44-7	dimethylcarbamoyl chloride	1B	1B	na	1B	1B/2	C
75-02-5	fluoroethylene	1B	1B	na	1B	1B/2	NO
556-52-5	2,3-epoxypropan-1-ol; glycidol; oxiranemethanol	1B	1B	na	2	1B/2	NO
96-09-3	styrene oxide; (epoxyethyl)benzene; phenyloxirane	1B	1B	na	2	1B/2	NO
79-01-6	trichloroethylene; trichloroethene	1B	1A	1A	1B	1A	C

126-72-7	tris(2,3-dibromopropyl) phosphate	1B	1B	na	na	1B/2	NO
7758-97-6	lead chromate	1B	1A	1A	1A	1A	C
1344-37-2	lead sulfochromate yellow; C.I. Pigment Yellow 34; [This substance is identified in the Colour Index by Colour Index Constitution Number, C.I. 77603.]	1B	1A	1A	1A	1A	C
12656-85-8	lead chromate molybdate sulfate red; C.I. Pigment Red 104; [This substance is identified in the Colour Index by Colour Index Constitution Number, C.I. 77605.]	1B	1A	1A	1A	1A	C
1333-82-0	chromium (VI) trioxide	1A	1A	1A	1A	1A	C
na	acids generated from chromium trioxide and their oligomers	1A	1A	1A	1A	1A	C
na	oligomers of chromic acid and dichromic acid	1A	1A	1A	1A	1A	C
7738-94-5	chromic acid	1B	1A	1A	1A	1A	C
13530-68-2	dichromic acid	1B	1A	1A	1A	1A	C
10588-01-9, 7789-12-0	sodium dichromate	1B	1A	1A	1A	1A	C
7778-50-9	potassium dichromate	1B	1A	1A	1A	1A	C
7789-09-5	ammonium dichromate	1B	1A	1A	1A	1A	C
7789-00-6	potassium chromate	1B	1A	1A	1A	1A	C
7775-11-3	sodium chromate	1B	1A	1A	1A	1A	C
234-329-8	potassium hydroxyoctaoxodizincatedichromate	1A	1A	1A	1A	1A	C
49663-84-5	pentazinc chromate octahydroxide	1A	1A	1A	1A	1A	C
95-53-4	o-toluidine; 2-aminotoluene	1B	1A	na	2	1A	C
95-69-2	4-chloro-o-toluidine [1] 4-chloro-o-toluidine hydrochloride [2]	1B	1B	na	na	1B/2	NO
92-87-5	benzidine; 1,1'-biphenyl-4,4'-diamine; 4,4'-diaminobiphenyl; biphenyl-4,4'-ylenediamine	1A	1A	1A	1A	1A	C
91-59-8	2-naphthylamine	1A	1A	na	1A	1A	C
92-67-1	biphenyl-4-ylamine; xenylamine; 4-aminobiphenyl	1A	1A	na	1A	1A	C
12070-12-1	tungsten carbide	na	1B	na	1B	1B/2	NO
7440-48-4	cobalt	1B	1B	na	2	1B/2	NO
7440-38-2	arsenic	1A	1A	1A	1A	1A	C
na	arsenic compounds, with the exception of those specified elsewhere in ANNEX VI CLP-ATP 18	na	1A	1A	1B	1A	C
7440-41-7	beryllium	1B	1A	1B	1A	1A	C
na	beryllium compounds with the exception of aluminium beryllium silicates, and with those specified elsewhere in this Annex	1B	1A	1B	1B	1A	C

7440-43-9	cadmium (pyrophoric)	1B	1A	1B	1B	1A	C
7440-43-9 [1] 1306-19-0 [2]	cadmium (non-pyrophoric) [1] cadmium oxide (non-pyrophoric) [2]	1B	1A	1B	1B	1A	C
7440-02-0	nickel	2	1B/2	NO	NO	1B/2	C
13463-39-3	tetracarbonylnickel; nickel tetracarbonyl	2	1A	1B	2	1A	C
12035-72-2	nickel subsulfide	1A	1A	1A	1A	1A	C
na	wood powder	na	1A	na	1A	1A	C
14808-60-7	quartz (SiO ₂)	1A	1A	na	1B	1A	C
na	soot	na	1A	na	na	1A	NO

CAS: Chemical Abstract Service Registry Number; **CLP:** Classification Labelling Packaging; **EPA:** Environmental Protection Agency (United States); **ACGIH:** American Conference of Governmental Industrial Hygienists (United States); **NTP:** National Toxicology Program (United States); **IARC:** International Agency for Research on Cancer; **NIOSH:** National Institute for Occupational Safety and Health (United States); C: carcinogen; NO: non carcinogen; Na: not available.

PART 4: GROUPS OF RESULTS

Table S5. 23 cases classified with concordance in all the classifications. In red, cases where were not used specific CAS, but CAS referred to a group of compounds.

CAS	CLP name	Note
1746-01-6	2,3,7,8-tetrachlorodibenzo[b,e][1,4]dioxin	CLP, EPA, AGIH classification not available
71-43-2	benzene	-
542-88-1	bis(chloromethyl) ether; oxybis (chloromethane)	-
12001-28-4; 132207-32-0; 12172-73-5; 77536-66-4; 77536-68-6; 77536-67-5; 12001-29-5	Asbestos [actinolite, amosite (grunerite), antofillite, crisotilo, crocidolite, tremolite]	-
75-01-4	vinyl chloride; chloroethylene	-
1327-53-3	diarsenic trioxide; arsenic trioxide	if not found, we have decided to use the classification of arsenic and its inorganic compounds
1303-28-2	diarsenic pentaoxide; arsenic pentoxide; arsenic oxide	if not found, we have decided to use the classification of arsenic and its inorganic compounds
na	arsenic acid and its salts with the exception of those specified elsewhere in this Annex	if not found, we have decided to use the classification of arsenic and its inorganic compounds
11103-86-9	zinc chromates including zinc potassium chromate	if not found, we have decided to use the classification of hexavalent chromium group
27208-37-3	cyclopenta [c,d] pyrene	CLP, EPA, AGIH classification not available; if not found, we can consider it as Coal Tars and Coal-Tar Pitches
8001-58-9	creosote*	ACGIH classification not available; if not found, we can consider it as Coal Tars and Coal-Tar Pitches
65996-93-2	pitch, coal tar, high-temp.**	EPA classification not available
1333-82-0	chromium (VI) trioxide	if not found, we have decided to use the classification of hexavalent chromium group
na	acids generated from chromium trioxide and their oligomers	if not found, we have decided to use the classification of hexavalent chromium group
na	oligomers of chromic acid and dichromic acid	if not found, we have decided to use the classification of hexavalent chromium group
234-329-8	potassium hydroxyoctaoxodizincatedichromate	if not found, we have decided to use the classification of hexavalent chromium group
49663-84-5	pentazinc chromate octahydroxide	if not found, we have decided to use the classification of hexavalent chromium group
92-87-5	benzidine; 1,1'-biphenyl-4,4'-diamine; 4,4'-diaminobiphenyl; biphenyl-4,4'-ylenediamine	-

91-59-8	2-naphthylamine	EPA classification not available
92-67-1	biphenyl-4-ylamine; xenylamine;	4- EPA classification not available
7440-38-2	arsenic	-
12035-72-2	nickel subsulfide	if not found, we can consider Nickel metal and other compounds (as Ni)
na	wood powder	EPA classification not available

* The distillate of coal tar produced by the high temperature carbonization of bituminous coal. It consists primarily of aromatic hydrocarbons, tar acids and tar bases.

** The residue from the distillation of high temperature coal tar. A black solid with an approximate softening point from 30 °C to 180 °C (86 °F to 356 °F). Composed primarily of a complex mixture of three or more membered condensed ring aromatic hydrocarbons.

CAS: Chemical Abstract Service Registry Number; **CLP:** Classification Labelling Packaging; **EPA:** Environmental Protection Agency (United States); **ACGIH:** American Conference of Governmental Industrial Hygienists (United States); **NTP:** National Toxicology Program (United States); **IARC:** International Agency for Research on Cancer; **NIOSH:** National Institute for Occupational Safety and Health (United States); Na: not available.

Table S6. 60 cases that have at least one discordant classification.

CAS	CLP name
70-25-7	1-methyl-3-nitro-1-nitrosoguanidine
96-12-8	1,2-dibromo-3-chloropropane
1336-36-3	polychlorobiphenyls; PCB
106-89-8	1-chloro-2,3-epoxypropane; epichlorhydrin
50-00-0	formaldehyde
50-32-8	benzo[a]pyrene; benzo[def]chrysene
75-21-8	ethylene oxide; oxirane
127-18-4	tetrachloroethylene
107-06-2	1,2-dichloroethane; ethylene dichloride
101-14-4	2,2'-dichloro-4,4'-methylenedianiline; 4,4'-methylene bis(2-chloroaniline)
24613-89-6	dichromium tris(chromate); chromium III chromate; chromic chromate
7789-06-2	strontium chromate
98-87-3	α,α -dichlorotoluene; benzylidene chloride; benzal chloride
100-44-7	α -chlorotoluene; benzyl chloride
98-88-4	benzoyl chloride
53-70-3	dibenz[a,h]anthracene
191-30-0	dibenzo[def,p]chrysene; dibenzo[a,l]pyrene
90640-80-5	anthracene oil *
12510-42-8	erionite
650-017-00-8	RCF-Refractory Ceramic Fibres
96-18-4	1,2,3-trichloropropane
121-14-2	2,4-dinitrotoluene dinitrotoluene [2]

[1]

106-99-0	1,3-butadiene; buta-1,3-diene	
106-97-8	butane (containing $\geq 0,1$ % butadiene (203-450-8))	
75-28-5	isobutane (containing $\geq 0,1$ % butadiene (203-450-8))	
101-77-9	4,4'-diaminodiphenylmethane; 4,4'-methylenedianiline	
79-06-1	acrylamide; prop-2-enamide	
593-60-2	bromoethylene	
119-90-4	3,3'-dimethoxybenzidine; o-dianisidine	
2425-06-1	captafol (ISO); 1,2,3,6-tetrahydro-N-(1,1,2,2-tetrachloroethylthio)phthalimide	
77-78-1	dimethyl sulphate	
79-44-7	dimethylcarbamoyl chloride	
75-02-5	fluoroethylene	
556-52-5	2,3-epoxypropan-1-ol; glycidol; oxiranemethanol	
96-09-3	styrene oxide; (epoxyethyl)benzene; phenyloxirane	
79-01-6	trichloroethylene; trichloroethene	
126-72-7	tris(2,3-dibromopropyl) phosphate	
7758-97-6	lead chromate	
1344-37-2	lead sulfochromate yellow; C.I. Pigment Yellow 34**	
12656-85-8	lead chromate molybdate sulfate red; C.I. Pigment Red 104 ***	
7738-94-5	chromic acid	
13530-68-2	dichromic acid	
10588-01-9, 7789-12-0	sodium dichromate	
7778-50-9	potassium dichromate	
7789-09-5	ammonium dichromate	
7789-00-6	potassium chromate	
7775-11-3	sodium chromate	
95-53-4	o-toluidine; 2-aminotoluene	
95-69-2	4-chloro-o-toluidine [1] 4-chloro-o-toluidine hydrochloride [2]	
12070-12-1	tungsten carbide	
7440-48-4	cobalt	
na	arsenic compounds, with the exception of those specified elsewhere in ANNEX VI CLP-ATP 18	
7440-41-7	beryllium	
na	beryllium compounds with the exception of aluminium beryllium silicates, and with those specified elsewhere in this Annex	
7440-43-9	cadmium (pyrophoric)	
7440-43-9 [1]	cadmium (non-pyrophoric)	[1]
1306-19-0 [2]	cadmium oxide (non-pyrophoric) [2]	
7440-02-0	nickel	
13463-39-3	tetracarbonylnickel; nickel tetracarbonyl	
14808-60-7	quartz (SiO ₂)	
na	soot	

* A complex combination of polycyclic aromatic hydrocarbons obtained from coal tar having an approximate distillation range of 300 °C to 400 °C (572 °F to 752 °F). Composed primarily of phenanthrene, anthracene and carbazole.

** This substance is identified in the Colour Index by Colour Index Constitution Number, C.I. 77603.

*** This substance is identified in the Colour Index by Colour Index Constitution Number, C.I. 77605.

CAS: Chemical Abstract Service Registry Number; **CLP:** Classification Labelling Packaging; Na: not available.

Table S7. Case data for groups of compounds.

CAS	Nome CLP	Group of compounds
50-32-8	benzo[a]pyrene; benzo[def]chrysene	Coal Tars and Coal-Tar Pitches
1327-53-3	diarsenic trioxide; arsenic trioxide	Arsenic
1303-28-2	diarsenic pentaoxide; arsenic pentoxide; arsenic oxide	Arsenic
na	arsenic acid and its salts with the exception of those specified elsewhere in this Annex	Arsenic
24613-89-6	dichromium tris(chromate); chromium III chromate; chromic chromate	Chromium
7789-06-2	strontium chromate	Chromium
11103-86-9	zinc chromates including zinc potassium chromate	Chromium
53-70-3	dibenz[a,h]anthracene	Coal Tars and Coal-Tar Pitches
191-30-0	dibenzo[def,p]chrysene; dibenzo[a,l]pyrene	Coal Tars and Coal-Tar Pitches
27208-37-3	cyclopenta [c,d] pyrene	Coal Tars and Coal-Tar Pitches
90640-80-5	anthracene oil; [A complex combination of polycyclic aromatic hydrocarbons obtained from coal tar having an approximate distillation range of 300 °C to 400 °C (572 °F to 752 °F). Composed primarily of phenanthrene, anthracene and carbazole.]	Coal Tars and Coal-Tar Pitches
8001-58-9	creosote; [The distillate of coal tar produced by the high temperature carbonization of bituminous coal. It consists primarily of aromatic hydrocarbons, tar acids and tar bases.]	Coal Tars and Coal-Tar Pitches
7758-97-6	lead chromate	Chromium
1344-37-2	lead sulfochromate yellow; C.I. Pigment Yellow 34; [This substance is identified in the Colour Index by Colour Index Constitution Number, C.I. 77603.]	Chromium
12656-85-8	lead chromate molybdate sulfate red; C.I. Pigment Red 104; [This substance is identified in the Colour Index by Colour Index Constitution Number, C.I. 77605.]	Chromium
1333-82-0	chromium (VI) trioxide	Chromium
na	acids generated from chromium trioxide and their oligomers	Chromium
na	oligomers of chromic acid and dichromic acid	Chromium
7738-94-5	chromic acid	Chromium
13530-68-2	dichromic acid	Chromium
10588-01-9, 7789-12-0	sodium dichromate	Chromium
7778-50-9	potassium dichromate	Chromium
7789-09-5	ammonium dichromate	Chromium
7789-00-6	potassium chromate	Chromium
7775-11-3	sodium chromate	Chromium
234-329-8	potassium hydroxyoctaoxodizincatedichromate	Chromium
49663-84-5	pentazinc chromate octahydroxide	Chromium
13463-39-3	tetracarbonylnickel; nickel tetracarbonyl	Nickel
12035-72-2	nickel subsulfide	Nickel

CAS: Chemical Abstract Service Registry Number; **CLP:** Classification Labelling Packaging; **Na:** not available.

Table S8 . CLP COC and IARC, EPA, ACGIH, NTP, NIOSH converted CoCs of Butane and Isobutane.

CAS	CLP Name	CLP	IARC	EPA	ACGIH	NTP	NIOSH
106-97-8	Butane	NO					
106-97-8	Butane (containing $\geq 0,1$ % butadiene (203-450-8))	1A	NO	n.a.	n.a.	NO	NO
	Isobutane	NO					
75-28-5	Isobutane (containing $\geq 0,1$ % butadiene (203-450-8))	1A	NO	n.a.	n.a.	NO	NO

CAS: Chemical Abstract Service Registry Number ; **CLP:** Classification Labelling Packaging; **IARC:** International Agency for Research on Cancer; **EPA:** Environmental Protection Agency (United States); **NTP:** National Toxicology Program (United States); **ACGIH:** American Conference of Governmental Industrial Hygienists (United States); **NIOSH:** National Institute for Occupational Safety and Health (United States); NO: non carcinogen; n.a.: not available

Table S9. case history of cluster 3.

Agency	CAS	Name	CoC
NTP	65996-93-2	pitch, coal tar, high-temperature	NO
	8007-45-2		1A
NIOSH	65996-93-2	cadmium (pyrophoric)	NO
		cadmium dust	C

CAS: Chemical Abstract Service Registry Number; **NTP:** National Toxicology Program (United States); **NIOSH:** National Institute for Occupational Safety and Health (United States); NO: non carcinogen.

Table S10. Cluster 4, divisions

Case data 4.1: not present in the NIOSH list, other documentation is available, but it is not conclusive.		
CAS	CLP name	added documentation
1336-36-3	polychlorobiphenyls; PCB	https://www.cdc.gov/niosh/docs/86-111/default.html
12510-42-8	erionite	https://blogs.cdc.gov/niosh-science-blog/2011/11/22/erionite/
650-017-00-8	RCF-Refractory Ceramic Fibres	https://www.cdc.gov/niosh/updates/upd-06-12-06.html
Cluster 4.2: not present in the NIOSH list, these cases have added documentations, but not for the carcinogenicity.		
CAS	CLP name	
75-02-5	Fluoroethylene	
556-52-5	2,3-epoxypropan-1-ol; glycidol; oxiranemethanol	
100-44-7	α -chlorotoluene; benzyl chloride	
Cluster 4.3: not present in the NIOSH list and we have not found other NIOSH documentations.		
CAS	CLP name	
70-25-7	1-methyl-3-nitro-1-nitrosoguanidine	
98-88-4	benzoyl chloride	
96-09-3	styrene oxide; (epoxyethyl)benzene; phenyloxirane	
126-72-7	tris(2,3-dibromopropyl) phosphate	
95-69-2	4-chloro-o-toluidine 4-chloro-o-toluidine hydrochloride [2]	[1]
12070-12-1	tungsten carbide	
7440-48-4	cobalt	
n.a.	soot	
Cluster 4.4: not present in the NTP RoC list and/or we have not found other NTP documentations on occupational field.		
CAS	CLP name	
121-14-2	2,4-dinitrotoluene [1]; dinitrotoluene [2]	
100-44-7	α -chlorotoluene; benzyl chloride	
CAS: Chemical Abstract Service Registry Number ; CLP: Classification Labelling Packaging; NTP: National Toxicology Program (United States); NIOSH: National Institute for Occupational Safety and Health (United States).		

Table S11. CoCs – CLP converted of PCBs (PolyChlorinated Biphenyls), RCF (Refractory Ceramic Fibres) and erionite.

CAS	Name	CLP	IARC	EPA	ACGIH	NTP	NIOSH
1336-36-3	Polychlorobiphenyls (PCB)	n.a.	1A	1B	n.a.	1B/2	NO
12510-42-8	Erionite	1A	1A	n.a.	n.a.	1A	NO
650-017-00-8	Refractory Ceramic Fibres (RCF)	1B	2	1B	1B	1B/2	NO

CAS: Chemical Abstract Service Registry Number; CLP: Classification Labelling Packaging; IARC: International Agency for Research on Cancer; EPA: Environmental Protection Agency (United States); ACGIH: American Conference of Governmental Industrial Hygienists (United States); NTP: National Toxicology Program (United States); NIOSH: National Institute for Occupational Safety and Health (United States); NO: non carcinogen; n.a.: not available