Protective Action Criteria (PAC) Rev 24B based on 60-minute AEGLs, ERPGs, or TEELs for Chemicals of Concern

Introduction

This document provides a brief introduction to Revision 24B of the Protective Action Criteria (PAC) for chemicals of concern. It differs from Revision 24A in that the TEEL values for nitrogen listed in Rev. 24A have been withdrawn pending a review of these values. PAC values, including AEGLs, ERPGs, and Temporary Emergency Exposure Limits (TEELs), are provided for 3354 chemicals. **TEEL values are always subject to change**, being replaced by AEGLs or ERPGs when new values are published, and are updated approximately annually when different concentration-limit [e.g., Permissible Exposure Limits (PELs) or Threshold Level Values (TLVs)] or toxicity data are published. Additional chemicals for which PAC values are derived are added at the same time.

Table 1 is an alphabetical list of the chemicals substances and their Chemical Abstract Services Registry Numbers (CASRNs), as well as some of their physical constants. Columns providing dates of original derivation, last reviewed and last revised, as well as the reference sources used for PAC-derivation of each chemical, have also been added. These columns have not yet been completely populated. Columns providing the lowest value found for the lower explosive limit (LEL), in parts per million (ppm), and the National Fire Protection Agency (NFPA) Health Hazard Rating (HHR) have also been added.

Table 2 is an alphabetical list of the PAC values for these chemicals. For the most part, values are given in parts per million (ppm) for gases and volatile liquids and in milligrams per cubic meter (mg/m³) for particulate materials (aerosols) and nonvolatile liquids. The CASRNs for chemicals that have AEGLs are **bolded** in **larger font**. Chemicals having ERPGs but no AEGLs are **bolded**. The actual AEGL and ERPG values are similarly bolded. The final column in Table 2 provides information of interest in deriving PAC values for that chemical, as well as information on changes in the PAC values (e.g., "T-0 changed" and "T-3 changed" from "PAC Rev 23," where "T-0" and "T-3" stand for "TEEL-0" and "PAC-3").

Table 3 is a list of PAC values sorted by CASRNs in the same units (ppm or mg/m³) as Table 2. The other Tables should routinely be consulted for physicochemical information, whether PAC values have changed, and the "Source of PACs." As in the other tables, for chemicals that have AEGLs, their CASRNs and AEGL values are **bolded** in **larger font**. For chemicals with ERPGs but no AEGLs, their CASRNs and ERPG values are **bolded**.

Table 4 is an alphabetical list of the PAC values in mass per unit volume (mg/m³) with the ppm to mg/m³ conversion (carried out at 25 °C and 760 mm Hg) performed before rounding. This table includes a column which provides "Source of PACs" information.

The DOE-approved methodology¹ was used to obtain concentration-limit derived PAC values. Published toxicity parameters from RTECS², HSDB², SAX³, and other sources were used to derive PAC-2 and PAC-3 values for chemicals lacking concentration-limit hierarchy-based values. Concentration limit-based values are presented as given by the original source, but toxicity-based values are rounded down to powers of 10 of the bases 1, 1.25, 1.5, 2, 2.5, 3, 3.5, 4, 5, 6, or 7.5 (unless the derived value is within 5% of the limit above it, e.g., 290 is rounded to 300). Where applicable, conversion from ppm to mg/m³ is made before rounding.

Further revisions of this document will be issued as warranted.

The SCAPA website features a PAC/TEEL webpage (http://orise.orau.gov/emi/scapa/teels.htm) that provides links to PAC/TEEL products and related technical information. This includes links to

- PAC data tables in Adobe Acrobat (.pdf) and MS Excel formats on the DOE Health, Safety, and Security (HSS) Chemical Safety Program's PAC webpage at http://www.hss.energy.gov/HealthSafety/WSHP/chem_safety/teel.html.
- An on-line searchable PAC database at http://www.atlintl.com/DOE/teels/teel.html.
- Links to the most recent AEGL and ERPG data sets.
- Links to the published TEEL methodology¹.

Several SCAPA-approved improvements to the TEEL-derivation methodology have been made since the two TEEL methodology documents cited above were published. These are included in DOE-HBK-1046-2008, Temporary Emergency Exposure Limits: Methods and Practice¹, available online. Suggestions for improvement to DOE-HDBK-1046-2008, Temporary Emergency Exposure Limits: Methods and Practice, for chemicals to be added to the list, to the format of the database, and other comments are welcome. All chemicals for which PAC values are derived will be added to the list. Anyone desiring PAC values for chemicals not on the "PAC Rev 24A" list is asked to send the request to Douglas K. Craig and the PAC development team (pacdevelopment@listserv.orau.gov). A more comprehensive set of contact information (including phone numbers and alternate contacts) is available by clicking on the contact link found near the bottom of the SCAPA PAC/TEEL webpage (http://orise.orau.gov/emi/scapa/contacts.htm#teels).

Notes for Tables

The PAC data tables are derived from an Excel Workbook. This workbook has been considerably modified in that nearly all the Excel functions used to automatically calculate PAC values have been replaced by Visual Basic macros. This change reduced the size of the file by a factor of about five and made the process of adding new chemicals to the list much simpler.

Changes from previous TEEL Revisions are usually the consequence of the correction or addition of data and rigid adherence to the above automated methodology¹, any deviation from which is indicated. The physicochemical data given in these tables are extracted from various sources, not all of which are in agreement with each other. However, the differences are not usually large enough to be of concern in the conduct of safety analyses. All molecular weights (MW) are given to two decimal places. The primary sources of these data are References 2 (ChemBank), 3 (SAX), 4 (*NIOSH Pocket Guide to Chemical Hazards*), and 5 (Hawley's Condensed Chemical Dictionary).

Abbreviations used in the tables are defined in Appendix A. Hierarchy-based PAC Values are obtained by strict application of the methodology (described in Reference 1), except as noted below or indicated on Table 2. Stippled cells indicate estimated values.

Information Pertinent to the Derivation of Hierarchy-based PAC Values

The most recent available references for PELs⁶. TLVs⁷, Recommended Exposure Limits (RELs)⁴, Workplace Environmental Exposure Levels (WEELs)⁸, and German limits (MAKs)⁹ are used. The most convenient source for these values is *Guide to Occupational Exposure Values* – 2008⁹, published annually by the American Conference of Governmental Industrial Hygienists.

For particulate materials, limits used (in mg/m³) are for total dust, even though published limits are sometimes also given for the respirable fraction.

PNOS = Particulates Not Otherwise Specified. This TLV-time weighted average (TWA) value is for total dust, and the respirable fraction is assumed to be 30% of total concentration.

For substances that are in particulate form, all PAC values have been reduced to a maximum value of 500 mg/m³. This concentration constitutes an upper bound for a stable cloud of respirable dust. The reason for this is that the coagulation rate of particles is a function of the square of the number concentration. Higher concentrations are unstable.

Values are restricted by the value of the next higher category, e.g., PAC-1 is restricted by the PAC-2. Thus, the following applies: **TEEL-0** \leq **PAC-1** \leq **PAC-2** \leq **PAC-3**.

For a few chemicals whose ERPG-1 value was odor-based rather than toxicity-based, the PAC-1 value was adjusted to the PEL-short term exposure limit (STEL), TLV-STEL, or 3 x TLV-TWA value. Where applicable, this is indicated in the last column of Table 2.

In the absence of other concentration limits or appropriate toxicity data for a chemical, a few PAC values are based on British, Finnish, Russian, or other guidelines¹⁰.

The usual order of use of toxicity data for PAC-2 and/or PAC-3 is subordinate to human toxicity data for a particular chemical.

A few values depart from the usual guidelines and are estimates based on existing concentration limits (at other PAC values) and/or a comparison with similar chemicals and/or a review of available toxicity data. For example, the PAC-3 value for 1-Bromo-3-chloro-5,5-dimethylhydantoin is estimated from the toxicity-based PAC-3 for 3-Bromo-1-chloro-5,5-dimethylhydantoin.

The PAC values presented in these tables are toxicity-based. In order to alert users as to the potential for other hazards, special formatting is used in Table 2 to indicate the relationship of these values to the LEL of a chemical:

- 10% LEL < PAC < 50% LEL, value in **bold green italics**.
- 50% LEL < PAC < 100% LEL, value in bold underlined pink italics.
- PAC > LEL, value in <u>bold double underlined red italics</u>.

Further Information

Because of its length (over 1200 pages), "PAC Rev 24A" is not available as a bound hard copy document. For further information please contact Douglas K. Craig and the PAC development team (pacdevelopment@listserv.orau.gov). A more comprehensive set of contact information

(including phone numbers and alternate contacts) is available by clicking on the contact link found near the bottom of the SCAPA PAC/TEEL webpage (http://orise.orau.gov/emi/scapa/contacts.htm#teels).

References

- U.S. Department of Energy (DOE). (2008). Temporary Emergency Exposure Limits: Methods and Practice, DOE-HBK-1046-2008. Available at:http://www.hss.energy.gov/nuclearSafety/techstds/standard/hdbk1046/DOE-HDBK-1046-2008.pdf.
- 2. CHEM-BANK[™]. (December 2007, updated quarterly). Databanks of potentially hazardous chemicals: RTECS[®] U.S. Department of Health and Human Services (NIOSH) Compact disc Vol. Id:RT36. PP-0018-0073 (SilverPlatter). This CD also includes other data bases, all of which have been scanned for pertinent data if necessary. These include: OHMTADS, TSCA and IRIS US Environmental Protection Agency; CHRIS U.S. Department of Transportation (Coast Guard); HSDB U.S. Library of Medicine; NPG U.S. National Institute for Occupational Safety and Health (NIOSH), and ERG2004 [Transport Canada, U.S. Department of Transportation, Secretariat of Transport/Communications (Mexico)].
- 3. Lewis, R. J., Sr. (2005). Sax's Dangerous Properties of Industrial Materials (11th Edition). New York: John Wiley & Sons. This publication is now available as a CD ROM (from Wiley Environmental Science).
- 4. U.S. Department of Health and Human Services, Public Health Service, Centers for Disease Control (2005). *NIOSH Pocket Guide to Chemical Hazards*. The latest version is included in Reference 2 above.
- 5. Lewis, R. J., Sr. (2001). *Hawley's Condensed Chemical Dictionary* (14th Edition). New York: John Wiley & Sons. This publication is available as a CD ROM.
- 6. U.S. Code of Federal Regulations, Title 29 Labor, Part 1910.1000, Occupational Safety and Health Administration, Air Contaminants, Subpart Z: Toxic and Hazardous Substances. Tables Z-1, Z-2 and Z-3 (July 2006).
- 7. American Conference of Governmental Industrial Hygienists (ACGIH), (2008). 2008 TLVs® and BEIs® Threshold Limit Values for Chemical Substances and Physical Agents. Cincinnati, OH.
- 8. American Industrial Hygiene Association (AIHA). (2008). The AIHA 2008 Emergency Response Planning Guidelines and Workplace Environmental Exposure Level Guides Handbook. Fairfax, VA: AIHA Press.
- 9. American Conference of Governmental Industrial Hygienists. (2007). *Guide to Occupational Exposure Values 2008 (GOEV)*. Cincinnati, OH.
- 10. International Labor Office. (1991). *Occupational Exposure Limits for Airborne Toxic Substances* (3rd Edition): Values of Selected Countries prepared from the ILO-CIS Data Base of Exposure Limits. Geneva.

<u>Definition of PACs (AEGLs, ERPGs or TEELs):</u>

Acute Exposure Guideline Levels (AEGLs) are intended to describe the risk to humans resulting from once-in-a-lifetime, or rare, exposure to airborne chemicals. They are defined as follows:

- AEGL-1 is the airborne concentration (expressed as ppm [parts per million] or mg/m³ [milligrams per cubic meter]) of a substance above which it is predicted that the general population, including susceptible individuals, could experience discomfort, irritation, or certain asymptomatic nonsensory effects. However, these effects are not disabling and are transient and reversible upon cessation of exposure.
- AEGL-2 is the airborne concentration (expressed as ppm or mg/m³) of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.
- AEGL-3 is the airborne concentration (expressed as ppm or mg/m³) of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

Emergency Response Planning Guidelines (ERPGs) are defined as follows:

- ERPG-1 is the maximum concentration in air below which it is believed nearly all
 individuals could be exposed for up to one hour without experiencing other than mild
 transient adverse health effects or perceiving a clearly defined objectionable odor.
- ERPG-2 is the maximum concentration in air below which it is believed nearly all
 individuals could be exposed for up to one hour without experiencing or developing
 irreversible or other serious health effects or symptoms that could impair their abilities to
 take protective action.
- ERPG-3 is the maximum concentration in air below which it is believed nearly all individuals could be exposed for up to one hour without experiencing or developing lifethreatening health effects.

Temporary Emergency Exposure Limits (TEELs) are defined as follows:

- TEEL-0 is the threshold concentration below which most people will experience no adverse health effects.
- TEEL-1 is the airborne concentration (expressed as ppm [parts per million] or mg/m³ [milligrams per cubic meter]) of a substance above which it is predicted that the general population, including susceptible individuals, could experience discomfort, irritation, or certain asymptomatic, nonsensory effects. However, these effects are not disabling and are transient and reversible upon cessation of exposure.
- TEEL-2 is the airborne concentration (expressed as ppm or mg/m³) of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting, adverse health effects or an impaired ability to escape.

■ TEEL-3 is the airborne concentration (expressed as ppm or mg/m³) of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

TEELs are intended for use until AEGLs or ERPGs are adopted for chemicals.

APPENDIX A. Key to Abbreviations

abs	absolute
ACGIH	American Conference of Governmental Industrial Hygienists
AEGL	Acute Exposure Guideline Level
af	atomic formula
AIHA	American Industrial Hygiene Association
alc	alcohol
alk	alkaline
amorph	amorphous
anhyd	anhydrous
approx	approximately
aq	aqueous
atm	atmosphere
autoign	auto-ignition
aw	atomic weight
BEI	ACGIH Biological Exposure Indexes
BP, bp	boiling point
b range	boiling range
CASRN	Chemical Abstracts Service Registry Number
CC	cubic centimeter
CC	closed cup
CL	ceiling concentration
COC	Cleveland open cup
conc	concentration, concentrated
compd(s)	compounds
contg	containing
cryst, crys	crystal(s), crystalline
d	density
D	day(s)
decomp, dec	decomposition
deliq	deliquescent
dil	dilute
DOT	U.S. Department of Transportation
EPA	U.S. Environmental Protection Agency
ERPG	Emergency Response Planning Guidelines of the AIHA
eth	ether
expls	explodes
(F)	Fahrenheit
FCC	Food Chemical Codex

FDA	U.S. Food and Drug Administration
fibrs	fibers
flam	flammable
flash p	flash point
FP, fp	freezing point
g, gm.	gram
glac	glacial
gran	granular, granules
hygr	hygroscopic
H, hr	hour(s)
HR	Hazard Rating (SAX)
htd	heated
htg	heating
IARC	International Agency for Research on Cancer
immisc	immiscible
incomp	incompatible
insol	insoluble
IU	International Unit
kg	kilogram (one thousand grams)
L,I	liter
LEL	Lower Explosive Limit
liq	liquid
M	minute(s)
m ³	cubic meter
mf	molecular formula
mg	milligram
misc	miscible
μ	micron
mL, ml	milliliter
mm	millimeter
mm Hg	pressure in millimeters of mercury
mod	moderately
MP, mp	melting point
mppcf	million particles per cubic foot
MW, mw	molecular weight
ng	nanogram
NIOSH	National Institute for Occupational Safety and Health
nonflam	nonflammable

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NTP	National Toxicology Program
OBS	obsolete
ОС	open cup
org	organic
OSHA	Occupational Safety and Health Administration
Pa	Pascals
PEL	permissible exposure level
petr	petroleum
pg	picogram (one trillionth of a gram)
Pk	peak concentration
pmole	picomole
powd	powder
ppb	parts per billion (v/v)
pph	parts per hundred (v/v)(percent)
ppm	parts per million (v/v)
ppt	parts per trillion (v/v)
prep	preparation
press	under pressure
PROP	properties
Pwdr	powder
rhomb	rhombic
SAX Number	each chemical's identifying code as used in SAX3
SCAPA	Subcommittee on Consequence Assessment and Protective Actions
S, sec	second(s)
SAR	Structure Activity Relationships
Si, sit, sitly	slightly
SG	specific gravity
sol	soluble
soln	solution
solv(s)	solvent(s)
spont	spontaneously
STEL	short term exposure limit

subl	sublimes
Т	PAC/TEEL
TCC	Tag closed cup
tech	technical
TEEL	Temporary Emergency Exposure Limits
temp	temperature
μ, u	micron
TLV	Threshold Limit Value
тос	Tag open cup
TWA	time weighted average
U, unk	unknown, unreported
UEL, uel	upper explosive limit
μg, ug	microgram
ULC, ulc	Underwriters Laboratory Classification
USDA	U.S. Department of Agriculture
vac	vacuum
vap	vapor
vap d	vapor density
VP, vap press	vapor pressure
Vol	volume
visc	viscosity
vsol	very soluble
W	week(s)
Υ	year(s)
%	percent(age)
>	greater than
<	less than
<=	equal to or less than
>=	equal to or greater than
•	degrees
°C	temperature in Celsius
(F), °F	temperature in Fahrenheit