

Protective Action Criteria (PAC) Rev 23 based on AEGLs, ERPGs, or TEELs for Chemicals of Concern 2007

PACs Rev 23 – August 2007

Introduction

This document provides a brief introduction to Revision 23 (PACs Rev 23 – August 2007) of the Protective Action Criteria (PACs) for chemicals of concern. It differs from Revision 22 in that several duplicate entries have been deleted, six chemicals for which AEGLs have been changed from “interim” to “final” status are so indicated, and a few chemicals have been added. PACs for oxygen have been withdrawn. The accompanying tables now include all chemicals for which Final or Interim Acute Exposure Guideline Levels (AEGLs) and Emergency Response Planning Guidelines (ERPGs) have been published to date¹, as well as Temporary Emergency Exposure Limits (TEELs). PAC values are provided for 3,316 chemicals. **TEEL values are always subject to change**, being replaced by AEGLs or ERPGs when new values are published, and updated approximately annually when different concentration-limit (e.g., permissible exposure limits (PELs) or threshold limit values (TLVs)) or toxicity data are published. Additional chemicals for which PACs 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 (CAS RNs), as well as some of their physical constants.

Table 2 is an alphabetical list of the PACs for these chemicals. 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. Chemicals having **AEGLs** are **bolded in larger font**. Chemicals having **ERPGs**, but no AEGLs, are **bolded**.

Table 3 is a list of PACs sorted by CAS RNs in the same units (ppm or mg/m³) as Table 2. The other Tables should routinely be consulted for physicochemical information, whether the PACs are AEGLs or ERPGs, and the “Source of PACs.”

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

PAC values that have been changed since the “TEELs Rev 21” are indicated in the last column of Table 2 (e.g., “T-1, T-3 changed”; where “T-1” and “T-3” stand for “TEEL-1” and “TEEL-3”). Chemicals added since publication of “TEELs Rev 21” are indicated.

The DOE SCAPA-approved methodology² was used to obtain concentration-limit derived PACs. Published toxicity parameters from RTECS³, HSDB³, SAX⁴, and other sources were used to derive PAC-2 and PAC-3 values for chemicals lacking concentration-limit hierarchy-based values, as documented in a Westinghouse Savannah River Company Technical Report (WSRC-TR-98-00080)⁵ and in “Derivation of Temporary Emergency Exposure Limits (TEELs)”⁶. 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 Subcommittee on Consequence Assessment and Protective Action (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 methodology^{5,6}.

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 a soon-to-be-published DOE-OEM document "Temporary Emergency Exposure Limits: Methods and Practice." Suggestions for improvement of this document, for chemicals to be added to the list, to the format, and other comments, are welcome. All chemicals for which PACs are derived will be added to the list. Anyone deriving PACs for chemicals not on the "PACs Rev 23" list using the published methodology is asked to send these to Douglas K. Craig (craigdk@earthlink.net). 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.

Notes for Tables

The PAC data tables are derived from an Excel Workbook. This workbook has been considerably modified from that described in detail in reference 5, in that nearly all the Excel functions used to automatically calculate PACs 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.

Chemicals whose names and CAS RNs are boldface are chemicals for which there are official AEGLs and/or ERPGs. "Added" means that the chemical has been added since "TEELs Rev 21." If a PAC value (AEGL, ERPG, or TEEL) has been changed in "PACs Rev 23" from previously published values, the affected values are indicated in the last column of Table 2 (e.g., "T-1, T-3 changed"). Changes from previous TEEL Revisions are usually the consequence of the correction or addition of data and rigid adherence to the above automated methodology^{5,6}, any deviation from which is indicated. The physicochemical data given in these tables is 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 3 (ChemBank), 4 (SAX), 7 (NIOSH), and 8 (Lewis).

Abbreviations used in the tables are defined in Appendix A, **Hierarchy-based PAC values**, are obtained by strict application of the methodology (described in references 2, 5, and 6), 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 Permissible Exposure Limits (PELs)⁹, Threshold Limit Values (TLVs)¹⁰, Recommended Exposure Limits (RELs)⁷, Workplace Environmental Exposure Levels (WEELs)¹ and German limits (MAKs)¹¹ are used. The most convenient source for these values is "Guide to Occupational Exposure Values - 2007"¹¹, compiled by the American Conference of Governmental Industrial Hygienists and updated annually.

For particulate materials, limits used (in mg/m³) are for total dust, even though 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 hierarchy-based PAC/TEEL for the next higher category, e.g., PAC-1 is restricted by the PAC-2 so that **TEEL-0 ≤ PAC-1 ≤ PAC-2 ≤ PAC-3** (this is the reason for withdrawal of PACs for oxygen).

For a few chemicals whose ERPG-1 value was odor-based, rather than toxicity-based, the PAC-1 value was adjusted to the PEL-STEEL, TLV-STEEL, 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 values are based on British, Finnish, Russian, or other guidelines¹².

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 PACs 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 lower explosive limit (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 bold double underlined *red italics*.

Further Information

Because of its length (nearly 1,100 pages), "PACs Rev 23" is not available as a bound hard copy document. For further information please contact Douglas K. Craig (craigdk@earthlink.net). 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.

References

1. The *AIHA 2007 Emergency Response Planning Guidelines and Workplace Environmental Exposure Level Guides Handbook*. AIHA Press, Fairfax, Virginia (2007).
2. Craig, D.K., J.S. Davis, R. DeVore, D.J. Hansen, A.J. Petrocchi, and T.J. Powell. Alternative Guideline Limits for Chemicals without ERPGs. *Amer. Ind. Hyg. Assoc. J.* 56, 919-925 (1995).
3. CHEM-BANK™ (June 2007, updated quarterly). Databanks of potentially hazardous chemicals: RTECS^R – 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. DOT, Secretariat of Transport/Communications [Mexico]).
4. Lewis, R.J., Sr. *Sax's Dangerous Properties of Industrial Materials*, 11th Edition, John Wiley & Sons, New York, (2005) (SAX). This publication is now available as a CD ROM (from Wiley Environmental Science).
5. Craig, D.K., and C. Ray Lux. WSRC-TR-98-00080. Methodology for Deriving Temporary Emergency Exposure Limits (TEELs) (U). Westinghouse Savannah River Company, Aiken, SC (1998).
6. Craig, D.K., J.S. Davis, D.J. Hansen, A.J. Petrocchi, T.J. Powell, and T.E. Tuccinardi, Jr. Derivation of Temporary Emergency Exposure Limits. *J. Appl. Toxicol.* 20, 11-20 (2000).
7. *NIOSH Pocket Guide to Chemical Hazards*. U.S. Department of Health and Human Services, Public Health Service, Centers for Disease Control (September 2005). The latest version is included in reference 3 above.
8. Lewis, R.J., Sr. *Hawley's Condensed Chemical Dictionary*, 14th Ed. John Wiley & Sons, New York (2001). This publication is available as a CD ROM.
9. 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).
10. 2007 TLVs^R and BEIs^R Threshold Limit Values for Chemical Substances and Physical Agents: The American Conference of Governmental Industrial Hygienists (ACGIH), Cincinnati, OH (2007).
11. *Guide to Occupational Exposure Values – 2007*. Compiled by the American Conference of Governmental Industrial Hygienists, Cincinnati, OH (2007).

12. Occupational Exposure Limits for Airborne Toxic Substances. Third Edition: Values of Selected Countries prepared from the ILO-CIS Data Base of Exposure Limits, International Labor Office, Geneva (1991).

Definition of PACs (AEGLs, ERPGs or TEELs)

Acute Exposure Guideline Levels (AEGLs) are defined as follows:

AEGL-1 is the airborne concentration (expressed as ppm [parts per million] or mg/m^3 [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/m^3) 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/m^3) 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 life-threatening 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 -- Same as ERPG-1 (with the exception of the recommended averaging time)

TEEL-2 -- Same as ERPG-2 (with the exception of the recommended averaging time)

TEEL-3 -- Same as ERPG-3 (with the exception of the recommended averaging time)

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

It is recommended that for application of PACs, concentration at the receptor point of interest be calculated as the peak 15-minute TWA concentration. It should be emphasized that TEELs are default values, following the published methodology explicitly. The only judgment involved is that exercised in the extraction of data used to calculate the recommended TEELs.

APPENDIX A. Key to Abbreviations

abs	absolute	htd	heated
ACGIH	American Conference of Governmental Industrial Hygienists	htg	heating
af	atomic formula	IARC	International Agency for Research on Cancer
AIHA	American Industrial Hygiene Association	immisc	immiscible
alc	alcohol	incomp	incompatible
alk	alkaline	insol	insoluble
amorph	amorphous	IU	International Unit
anhyd	anhydrous	kg	kilogram (one thousand grams)
approx	approximately	L,l	liter
aq	aqueous	LEL, lel	lower explosive limit
at, atm	atmosphere	liq	liquid
autoign	auto-ignition	M	minute(s)
aw	atomic weight	m ³	cubic meter
BEI -	ACGIH Biological Exposure Indexes	mf	molecular formula
BP, bp	boiling point	mg	milligram
b range	boiling range	misc	miscible
CAS RN	Chemical Abstracts Service Registry Number	μ, u	micron
cc	cubic centimeter	mL, ml	milliliter
CC	closed cup	mm.	millimeter
CL	ceiling concentration	mmHg	pressure in millimeters of mercury
COC	Cleveland open cup	mod	moderately
conc	concentration, concentrated	MP, mp	melting point
compd(s)	compounds	mppcf	million particles per cubic foot
contg	containing	MW, mw	molecular weight
cryst, crys	crystal(s), crystalline	ng	nanogram
d	density	NIOSH	National Institute for Occupational Safety and Health
D	day(s)	nonflam	nonflammable
decomp, dec	decomposition	NTP	National Toxicology Program
deliq	deliquescent	OBS	obsolete
dil	dilute	OC	open cup
DOT	U.S. Department of Transportation	org	organic
EPA	U.S. Environmental Protection Agency	OSHA	Occupational Safety and Health Administration
ERPG	Emergency Response Planning Guidelines of the AIHA	Pa	Pascals
eth	ether	PEL	permissible exposure limit
expls	explodes	petr	petroleum
(F)	Fahrenheit	pg	picogram (one trillionth of a gram)
FCC	Food Chemical Codex	Pk	peak concentration
FDA	U.S. Food and Drug Administration	pmole	picomole
fibrs	fibers	powd	powder
flam	flammable	ppb	parts per billion (v/v)
flash p	flash point	pph	parts per hundred (v/v)(percent)
FP, fp	freezing point	ppm	parts per million (v/v)
g, gm.	gram	ppt	parts per trillion (v/v)
glac	glacial	prep	preparation
gran	granular, granules	press	under pressure
hygr	hygroscopic	PROP	properties
H, hr	hour(s)	Pwdr	powder
HR	Hazard Rating (SAX)	rhomb	rhombic

SAX Number	each chemical's identifying code as used in SAX3	U, unk	unknown, unreported
SCAPA	Subcommittee on Consequence Assessment and Protective Actions	UEL, uel	upper explosive limit
S, sec	second(s)	µg, ug	microgram
SAR	Structure Activity Relationships	ULC, ulc	Underwriters Laboratory Classification
Si, sit, sitly	slightly	USDA	U.S. Department of Agriculture
SG	specific gravity	vac	vacuum
sol	soluble	vap	vapor
soln	solution	vap d	vapor density
solv(s)	solvent(s)	VP, vap press	vapor pressure
spont	spontaneously	Vol	volume
STEL	short term exposure limit	visc	viscosity
subl	sublimes	vsol	very soluble
T	PAC/TEEL	W	week(s)
TCC	Tag closed cup	Y	year(s)
tech	technical	%	percent(age)
TEEL	Temporary Emergency Exposure Limits	>	greater than
temp	temperature	<	less than
µ, u	micron	< =	equal to or less than
TLV	Threshold Limit Value	> =	equal to or greater than
TOC	Tag open cup	°	degrees
TWA	time weighted average	°C	temperature in Celsius (Centigrade)
		(F), °F	temperature in Fahrenheit