A NEW STANDARD OF ABBREVIATIONS FOR BROMINATED, CHLORINATED AND PHOSPHORUS CONTAINING FLAME RETARDANTS

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Introduction

The number of environmental contaminants has increased dramatically over the past 50 years. One group of chemicals of concern is flame retardants (FRs) such as brominated-, chlorinated- and phosphorous FRs (BFRs, CFRs and PFRs). The European Food Safety Agency (EFSA) has over the last two years produced five hitherto adopted EFSA opinions [1-5] and one more is under way. These documents deals with food and feed exposure and the toxicity of the BFRs discussed, i.e. PBBs[1], PBDEs[2], HBCDDs[3], TBBPA[4] and its derivatives, phenolic BFRs including their derivatives (not TBBPA)[5] and the final document deals with emerging and novel neutral BFRs. In addition, Eljarrat and Barceló edited in 2011 a book on BFRs[6].

The large number of established, emerging, potential and novel FRs and the increasing number of publications dealing with all of those call for harmonized and simple abbreviations to avoid confusion in the area. In the literature it is not uncommon to find that several abbreviations is used to describe the same chemical or that one abbreviation may even be used to describe two different chemicals. In a recent article[7], we propose abbreviations for halogenated and organophosphorus FRs using a two step procedure to establish Practical Abbreviations (PRABs). In the first step, Structured Abbreviations (STABs) are derived using specific STAB criteria based on the chemical structure of the FR. The STABs are helpful since they give useful information about the FRs structure. However, since some of the STABs are complicated and long, we proposed instead the use of the shorter PRABs. The PRABs are in most cases derived from the STAB, although, we also consider abbreviations extensively used in previous literature. This presentation will give the rational for how to derive STABs and also present the PRABs we propose for future use.

Materials and methods

STABs are prepared on basis of defined abbreviations for functional groups, numbers of substituents, prefixes and other molecular specific descriptors. These are listed in Table 1. A few examples are given on how to construct STABs in the "Result and discussion" part below.

PRABs, with some specific exceptions, are constructed on basis of the STABs, but with the aim to reach simplified forms to write, present and discuss. The PRABs are written with capital letters. For a number of established BFRs we have chosen to stick to the well-known and generally accepted abbreviations. Examples of a few PRABs are given in the "Result and discussion" part below.

Table 1. Abbreviations of element, functional groups, molecular fragments and similar entities in a molecule, numbering and prefixes to be applied when constructing structured abbreviations (STABs) of BFRs, CFRs and PFRs.

Element, Functional group, Molecular fragment abbreviations					
Letter	**Group**	**Letter**	**Group**	**Letter**	**Group**
A	Allyl	Ac	Acetate	Acr	Acrylate
AE	Allyl ether	Anh	Anhydride	Ant	Anthracene
B	Bromine	Bn	Benzyl	BnB	Benzylbromide
BnC	Benzylchloride	Bu	Butane or butyl	BuO	Butoxy
Bz	Benzo or benzene	Bzo	Benzoate		
C	Chlorine	Ca	Carboxylic acid		
DD	Dodecane or dodecyl	De	Decane or decyl	Den	Decen
E	Ether	Et	Ethane or ethyl	EtO	Ethoxy
F	Furan				
GE	Glycidyl ether				
H	Hexane or hexyl	Ht	Heptane or heptyl	Hte	Hepten
Im	Imide	In	Indane		
Me	Methane or methyl				
N	Nonane or nonyl				
O	Octane or octyl	OH	Hydroxyl	OPO	Oxaphosphorinoxide
P	Poly – if first in abbreviation Phosphate- if last in abbreviation	Ph	Phenol or phenyl	PhO	Phenoxy
Pht	Phthalate	Pr	Propane or propyl	Prt	Propionate
Pt	Pentane or pentyl				
Re	Resorcinol				
Sty	Styrene				
T	Toluene	Taz	Triazine	Tazto	Triazine-trione

Numbering of substituents						
Di for 2	Tr for 3	Te for 4	Pe for 5	Hx for 6	Hp for 7	O for 8
N for 9	D for 10	UD for 11	DD for 12	TrD for 13	TeD for 14	PeD for 15

Prefices						
c for cyclo	bc for bicyclo	i for iso	b for bis	t for tris		

Results and discussion

Very few of all BFRs, CFRs and PFRs may be discussed in terms of being really well known with extensive scientific reports on production, use, occurrence, (eco-)toxicity, health and environmental effects. However, for these few FRs we may list them under a heading: *Established flame retardants* (e.g. PBBs, PBDEs, TBBPA, HBCDD). *Emerging FRs* makes up a far larger group of chemicals, being defined as FRs that have been reported to occur in any abiotic compartment or in biota, incl. humans. *Novel FRs* are then those that so far only have been shown to be used or present in materials and goods. Finally, chemicals only indicated in the literature or in patents to have properties making them useful as flame retardants are defined as *Potential FR*s. By listing all of these BFRs, CFRs and PFRs we have listed 55, 16 and 23 individual or groups thereof, respectively[7].

In this context we only want to point out the need for common abbreviations to be used by the scientific community and other stakeholders to promote communication regarding flame retardants. It became very clear to us in the process of developing useful abbreviations that a tired procedure is necessary. Hence the process of developing STABs always starts with looking into the chemical structure of the compound and which name this compound may be listed with. The common structural elements, functional groups and atoms need to be handled

similarly each time they show up in new FR and similarly the numbering and prefixes need to be handled similarly. Accordingly the STAB and also later on the PRAB of e.g. tris(2,3-dichloropropyl) phosphate and tris(1,3-dichloropropyl) phosphate must be different. Accordingly the STABs of these two PFRs are: tDiCiPP and tDiCPrP, respectively. Making these two STABs into PRABs leave us with TDCIPP and TDCPP, respectively.

The link between the STABs and PRABs are quite obvious for the many of the BFRs, e.g. the STAB: TeBCT for tetrabromochlorotoluene with the PRAB: TBCT; the STAB: TBBPA-bDiBPrE for tetrabromobisphenol A bis(2,3-dibromopropyl) ether with the PRAB: TBBPA-BDBPE. However for some BFRs the STABs become quite complicated, as in case of the compound: 5,6-Dibromo-1,10,11,12,13,13-hexachloro-11-tricyclo[8.2.1.02,9]tridecene, generating a STAB: DiBHxC-TrcTrDen and from there we suggest a PRAB: DBHCTD (see Bergman et al. [7] for further details).

The PRABs of all identified BFRs are given in Table 2, while we want to refer to the original publication[7] for PRABs and all other information regarding how to construct STABs and PRABs.

Table 2. Practical abbreviations (PRABs) of Established, Emerging, Novel and Potential BFRs. Two compounds are rated as "BFR related compounds". The BFRs are listed in alphabetical order under each sub-heading.

Established BFRs	**PRABs**
2,4-Dibromophenol	DBP
Hexabromocyclododecane	HBCDD (HBCD)
Polybrominated biphenyls	PBBs
Polybrominated diphenyl ethers	PBDEs
Tetrabromobisphenol A	TBBPA
2,4,6-Tribromophenol	TBP
Emerging BFRs	**PRABs**
Bis(2-ethylhexyl) tetrabromophthalate	BEH-TEBP
1,2-Bis(2,4,6-tribromophenoxy)ethane	BTBPE
Decabromodiphenyl ethane	DBDPE/BDPE-209
4-(1,2-Dibromoethyl)-1,2-dibromocyclohexane	DBE-DBCH
5,6-Dibromo-1,10,11,12,13,13-hexachloro-11-tricyclo[8.2.1.02,9]tridecene	DBHCTD
2-Ethylhexyl 2,3,4,5-tetrabromobenzoate	EH-TBB
Hexabromobenzene	HBB
1,2,3,4,7,7-Hexachloro-5-(2,3,4,5-tetrabromophenyl)-bicyclo[2.2.1]hept-2-ene	HCTBPH
Pentabromobenzyl acrylate	PBB-Acr
Pentabromoethylbenzene	PBEB
Pentabromophenol	PBP
Pentabromotoluene	PBT
Tetrabromobisphenol A bis(2,3-dibromopropyl) ether	TBBPA-BDBPE
Tetrabromobisphenol S bis(2,3-dibromopropyl ether)	TBBPS-BDBPE
1,2,5,6-Tetrabromocyclooctane	TBCO
2,3,4,5-Tetrabromo-6-chlorotoluene	TBCT
2,4,6-Tribromophenyl allyl ether	TBP-AE
2,4,6-Tribromophenyl 2,3-dibromopropyl ether	TBP-DBPE
1,2,4,5-Tetrabromo-3,6-dimethylbenzene	TBX
1,3,5-tris(2,3-dibromopropyl)-1,3,5-triazine-2,4,6-trione	TDBP-TAZTO

Novel BFRs	**PRABs**
1,3-bis(2,3-dibromopropyl)-5-allyl-1,3,5-Triazine-2,4,6(1H,3H,5H)-trione	BDBP-TAZTO
Decabromodibenzyl ether	DBDBE/BDBE-209
2,2-Bis(bromomethyl)-1,3-propanediol	DBNPG
1-(2,3-dibromopropyl)-3,5-diallyl-1,3,5-Triazine-2,4,6(1H,3H,5H)-trione	DBP-TAZTO
Dibromostyrene	DBS
N,N'-Ethylenebis(tetrabromophthalimide)	EBTBPI
Hexabromocyclodecane	HBCYD
2-(2-Hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromophthalate	HEEHP-TEBP
Octabromotrimethylphenyl indane	OBTMPI
Tetradecabromo-1,4-diphenoxybenzene	4'-PeBPO-BDE206
Tetrabromobisphenol A bis(allyl) ether	TBBPA-BAE
Tetrabromobisphenol A bis(2-hydroxyethyl) ether	TBBPA-BHEE
2,2,2-Tris(bromomethyl)ethanol	TBNPA
Tris(2,4,6-tribromophenoxy)-s-triazine	TBP-TAZ
Tris(2,3-dibromopropyl) phosphate	TDBPP
Tris[3-bromo-2,2-bis(bromomethyl)propyl] phosphate	TTBNPP
Potential BFRs	**PRABs**
Pentabromobenzyl bromide	PBBB
Pentabromobenzyl chloride	PBBC
Pentabromophenol allyl ether	PBP-AE
Tetrabromobisphenol A bisacrylate	TBBPA-BA
Tetrabromobisphenol A bis(glycidyl) ether	TBBPA-BGE
3,3',5,5'-Tetrabromobisphenol A bisacetate	TBBPA-BOAc
Tebrabromobisphenol A bispropanoate	TBBPA-BP
Tetrabromobisphenol S	TBBPS
3,4,5,6-Tetrabromophthalic anhydride	TBP-Anh
3-(Tetrabromopentadecyl)-2,4,6-tribromophenol	TBPD-TBP
BFR related compounds	**PRABs**
Tetrabromobisphenol A bismethyl ether	TBBPA-BME
Tetrabromobisphenol S bismethyl ether	TBBPS-BME

Acknowledgements
NVDE and AC acknowledge PhD and post-doctoral fellowships from the Flanders Research Foundation (FWO). AR acknowledges faculty funding from Stockholm University and Stockholm University's Strategic Marine Environmental Research Founds through the Baltic Ecosystem Adaptive Management (BEAM).

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