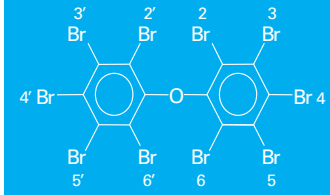
Polybrominated Diphenyl Ethers

Reference Mass Table

	# Br	m	Rel. Int	m+2	Rel. Int	m+4	Rel. Int	m+6	Rel. Int	m+8	Rel. Int	m+10	Rel. Int	m+12	Rel. Int	m+14	Rel. Int	Rel. Int M+/ [M-2Br]+
PBDE	1	247.9831	100.0	249.9812	98.3													100
Native	2	325.8936	51.1	327.8916	100.0	329.8897	49.4											100
M^+	3	403.8042	34.2	405.8021	100.0	407.8001	97.9	409.7983	32.4									100
	4	481.7147	17.5	483.7126	68.2	485.7106	100.0	487.7087	65.4	489.7068	16.3							100
	5			561.6232	51.2	563.6211	100.0	565.6191	97.8	567.6172	48.0							85
	6			639.5337	31.5	641.5316	76.8	643.5296	100.0	645.5276	73.4	647.5257	28.9					60
	7			717.4442	21.0	719.4421	61.5	721.4401	100.0	723.4381	97.7	725.4361	57.4	727.4342	18.9			55
	8					797.3526	42.1	799.3506	82.0	801.3486	100.0	803.3466	78.2	805.3446	38.3			50
	9					875.2632	30.1	877.2611	68.4	879.2591	100.0	881.2571	97.6	883.2551	63.6	885.2531	26.7	40
	10					953.1737	19.3	955.1716	50.1	957.1696	85.4	959.1676	100.0	961.1656	81.4	963.1636	45.5	25
PBDE	2	168.0570	100.0															
Native	3	245.9675	100.0	247.9655	98.3													
$[M-2Br]^+$	4	323.8780	51.1	325.8760	100.0	327.8741	49.4											95
	5	401.7885	34.2	403.7865	100.0	405.7845	97.9	407.7826	32.4									100
	6	479.6990	17.5	481.6970	68.2	483.6950	100.0	485.6930	65.4	487.6912	16.3							100
	7			559.6075	51.2	561.6055	100.0	563.6035	97.8	565.6015	48.0							100
	8			637.5180	31.5	639.5160	76.8	641.5140	100.0	643.5120	73.4	645.5100	28.9					100
	9			715.4285	21.0	717.4265	61.5	719.4245	100.0	721.4225	97.7	723.4205	57.4	725.4185	18.9			100
	10					795.3370	42.1	797.3350	82.0	799.3329	100.0	801.3309	78.2	803.3290	38.3			100

	# Br	m	Rel. Int	m+2	Rel. Int	m+4	Rel. Int	m+6	Rel. Int	m+8	Rel. Int	m+10	Rel. Int	m+12	Rel. Int	m+14	Rel. Int	Rel. Int M+/ [M-2Br]+
PBDE	1	260.0234	100.0	262.0214	97.5													100
$^{13}C_{12}$ Standard	2	337.9339	51.3	339.9319	100.0	341.9298	48.8											100
M^+	3	415.8444	34.2	417.8424	100.0	419.8403	97.4	421.8383	31.7									100
	4	493.7549	17.6	495.7529	68.5	497.7508	100.0	499.7488	65.0	501.7468	15.9							100
	5			573.6634	51.4	575.6614	100.0	577.6593	97.4	579.6573	47.5							85
	6			651.5739	31.7	653.5719	77.0	655.5698	100.0	657.5678	73.0	659.5657	28.5					60
	7			729.4844	21.1	731.4824	61.6	733.4803	100.0	735.4783	97.4	737.4763	56.9	739.4742	18.5			55
	8					809.3929	42.2	811.3908	82.2	813.3888	100.0	815.3868	77.9	817.3847	37.9			50
	9					887.3034	30.2	889.3014	68.5	891.2993	100.0	893.2973	97.3	895.2952	63.2	897.2932	26.4	40
	10					965.2139	19.4	967.2119	50.3	969.2098	85.6	971.2078	100.0	973.2057	81.1	975.2037	45.1	25
PBDE	2	180.0972	100.0															
$^{13}C_{12}$ Standard	3	258.0077	100.0	260.0057	97.5													
$[M-2Br]^+$	4	335.9182	51.3	337.9162	100.0	339.9142	48.8											95
	5	413.8288	34.2	415.8267	100.0	417.8247	97.4	419.8227	31.7									100
	6	491.7393	17.6	493.7372	68.5	495.7352	100.0	497.7332	65.0	499.7311	15.9							100
	7			571.6477	51.4	573.6457	100.0	575.6437	97.4	577.6416	47.5							100
	8			649.5583	31.7	651.5562	77.0	653.5542	100.0	655.5521	73.0	657.5501	28.5					100
	9			727.4688	21.1	729.4667	61.6	731.4647	100.0	733.4626	97.4	735.4606	56.9	737.4586	18.5			100
	10					807.3772	42.2	809.3752	82.2	811.3732	100.0	813.3711	77.9	815.3691	37.9			100



The calculated reference masses are based on the following values for isotopic masses:
^{1}H 1.0078250321u,
^{12}C 12.0000000000 u,
^{13}C 13.0033548378 u,
^{16}O 15.9949146221 u,
^{35}Cl 34.9688527100 u and
^{37}Cl 36.9659026000 u.
^{79}Br 78.9183376u and
^{81}Br 80.9162910u.

All listed masses refer to singly positively charged ions. The mass of the electron (0.000548579911u) was taken into account for the calculation of the ionic masses. Reference: Nuclear Phys. A 1995, 595, 409-480; J. Phys.

Chem. Ref. Data 1999, 28 (6), 1713-1852 and references cited therein.

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Polybrominated Diphenyl Ethers

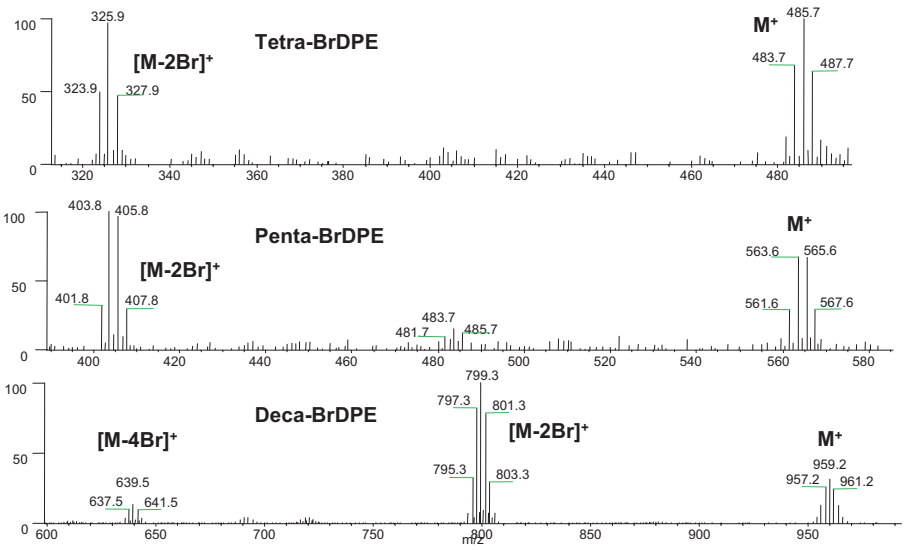
Reference Mass Table

Calibration Solutions

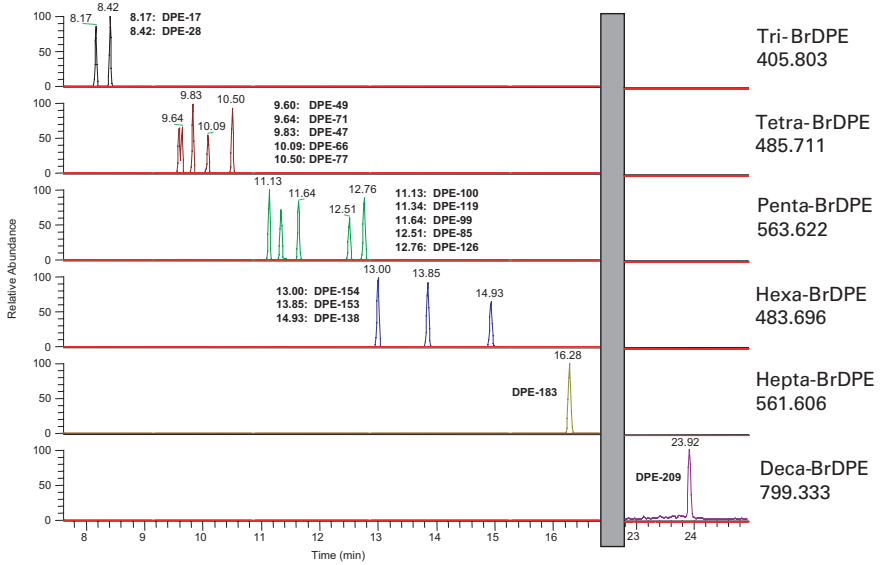
	CS1	CS2	CS3 [ng/ml]	CS4	CS5
Native PBDEs					
4-Bromodiphenyl ether (3)	1	5	20	100	400
2,4-Dibromodiphenyl ether (7)	1	5	20	100	400
4,4'-Dibromodiphenyl ether (15)	1	5	20	100	400
2,2',4-Tribromodiphenyl ether (17)	1	5	20	100	400
2,4,4'-Tribromodiphenyl ether (28)	1	5	20	100	400
2,2',4,4'-Tetrabromodiphenyl ether (47)	1	5	20	100	400
2,2',4,5'-Tetrabromodiphenyl ether (49)	1	5	20	100	400
2,3',4,4'-Tetrabromodiphenyl ether (66)	1	5	20	100	400
2,3',4',6-Tetrabromodiphenyl ether (71)	1	5	20	100	400
3,3',4,4'-Tetrabromodiphenyl ether (77)	1	5	20	100	400
2,2',3,4,4'-Pentabromodiphenyl ether (85)	1	5	20	100	400
2,2',4,4',5-Pentabromodiphenyl ether (99)	1	5	20	100	400
2,2',4,4',6-Pentabromodiphenyl ether (100)	1	5	20	100	400
2,3',4,4',6-Pentabromodiphenyl ether (119)	1	5	20	100	400
3,3',4,4',5-Pentabromodiphenyl ether (126)	1	5	20	100	400
2,2',3,4,4',5'-Hexabromodiphenyl ether (138)	1	5	20	100	400
2,2',4,4',5,5'-Hexabromodiphenyl ether (153)	1	5	20	100	400
2,2',4,4',5,6'-Hexabromodiphenyl ether (154)	1	5	20	100	400
2,2',3,4,4',5',6-Heptabromodiphenyl ether (183)	1	5	20	100	400
Decabromodiphenyl ether (209)	10	50	200	1000	4000

13C-Labelled PBDE Standards					
4-Bromo[$^{13}C_{12}$]diphenyl ether (3L)	100	100	100	100	100
4,4'-Dibromo[$^{13}C_{12}$]diphenyl ether (15L)	100	100	100	100	100
2,4,4'-Tribromo[$^{13}C_{12}$]diphenyl ether (28L)	100	100	100	100	100
2,2',4,4'-Tetrabromo[$^{13}C_{12}$]diphenyl ether (47L)	100	100	100	100	100
2,2',4,4',5-Pentabromo[$^{13}C_{12}$]diphenyl ether (99L)	100	100	100	100	100
2,2',4,4',5,5'-Hexabromo[$^{13}C_{12}$]diphenyl ether (153L)	100	100	100	100	100
2,2',4,4',5,6'-Hexabromo[$^{13}C_{12}$]diphenyl ether (154L)	100	100	100	100	100
2,2',3,4,4',5',6-Heptabromo[$^{13}C_{12}$]diphenyl ether (183L)	100	100	100	100	100
Decabromo[$^{13}C_{12}$]diphenyl ether (209L)	100	100	100	100	100
2,2',3,4,4',6'-Hexabromo[$^{13}C_{12}$]diphenyl ether (139L)	100	100	100	100	100

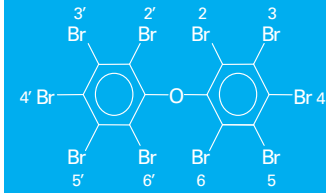
All concentrations are given for calibration solutions BDE-CVS-A as available from Wellington Laboratories Inc., Ontario, Canada.



Spectra acquired @ 40eV (source temperature 280 °C). With bromination degree higher than 4, the $[M\text{-}2Br]^+$ ion is more abundant than the M^+ ion. The fragmentation pattern is dependent on the ion source temperature.



Experimental conditions: EI, 40 eV, ion source temp. 280 °C, R = 10,000 (10 % valley), Ref.: PFK, GC: Trace GC Ultra, DB5ms (15/0.25/0.1), constant flow 1 mL/min, splitless injection (1 min), inj. Temp. 280 °C, oven program 120 °C/2 min – 230 °C/15 – 270 °C/5 – 330 °C/10, transfer line temp. 280 °C.



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