WELLINGTON LABORATORIES

Reference and Handling Guide

GC/MS CHARACTERIZATION AND ANALYSIS OF SELECTED HALOGENATED AROMATIC COMPOUNDS

GUIDELINES FOR THE USE AND HANDLING OF WELLINGTON PRODUCTS

HAZARDS

The majority of our products are halogenated aromatic hydrocarbons in solution in organic solvents such as nonane, toluene and isooctane. Although the maximum concentration is 100 µg/ml, that is 0.01% (w/v), these compounds must be considered toxic and potentially carcinogenic and should be handled accordingly.

With all of our products due care should be exercised to prevent human contact and ingestion. The absence of a toxicity warning for any of our products must not be interpreted as an indication that there is no possible health hazard.

NOTE:
THESE MATERIALS SHOULD ONLY BE USED BY PERSONNEL TRAINED IN THE HANDLING OF HAZARDOUS CHEMICALS.
ALL PROCEDURES SHOULD BE PERFORMED IN A FUME HOOD AND SUITABLE GLOVES, EYE PROTECTION AND CLOTHING SHOULD BE WORN AT ALL TIMES.

RECEIPT, INSPECTION, HANDLING AND STORAGE

Unless crystalline material is provided, all of our reference standard solutions come in flame-sealed, pre-scored amber glass ampoules. Upon receipt, inspect the ampoules for breakage and leakage and then store them upright until needed. The ampoules can be stored at ambient temperature until opened.

Prior to opening, allow the solution to drain into the bottom of the ampoule, lightly tapping the ampoule if necessary. Using the plastic ampoule collar provided, hold the ampoule upright and snap the top off, breaking away from the body.

Transfer the solution to an amber glass container that can be tightly sealed for storage. To prevent evaporation of the solvent, it is suggested that this solution, and subsequent mixtures and/or dilutions, be stored at refrigerator temperatures.

DISPOSAL

All waste materials generated during the use of these solutions should be treated as hazardous in accordance with national and regional regulations. A licensed disposal company should be employed. Some options for the destruction of these materials include high temperature incineration, photolysis or chemical treatment using reagents such as sodium naphthalene or KPEG reagent.

Literature references for some of these methods can be provided upon request.

ACCURACY

Each of our stock solutions is prepared from crystalline material that has been well characterized as to its structure and purity.

The crystalline material is weighed using microbalances that are externally calibrated using NIST-traceable weights. Solutions are prepared by completely dissolving the crystalline material in ultrapure, distilled-in-glass solvents. The volumetric flasks used for this purpose, and the pipets used for subsequent preparation of dilutions and mixtures, are all of class A tolerance and NIST-traceable.

The maximum percent relative combined uncertainty for solution preparation is calculated to be ± 5 %.

INTERLABORATORY CERTIFICATION

Wellington continues to submit its standards for independent interlaboratory testing and certification. Since 1991, our standards have been tested in over 20 international round-robins.

To date, solutions of the compounds listed below have been repeatedly tested and the approximate total number of analyses are given.

- 2,3,7,8 - substituted PCDDs and PCDFs .....1250 HRMS analyses
- Dioxin-like (WHO) PCB congeners.....1000 HRMS analyses
- PBDEs .....100 HRMS analyses

The overall averages of the data received for all of the compounds were found to be well within ± 10 % of the design values.

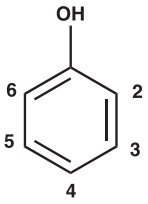
EXPIRY DATE/SHELF LIFE

In order to accurately determine the shelf life of products such as ours, testing must reveal significant degradation or loss in concentration of the particular analyte. In comparing freshly prepared solutions to older solutions by GC/MS, we have not detected any significant changes. Many of these older solutions were prepared and ampouled more than 15 years ago. Thus our stability studies, as they should, remain ongoing.

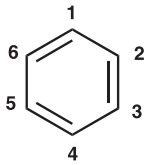
For our products where the expiry date on the certificate of analysis (CofA) states, “stability studies ongoing”, we consider that our reference standard solutions retain their accuracy for a period of 5 years from delivery in the unopened ampoule.

NOTE: The predominant degradation pathway for our compounds is likely photolysis and thus protection from light is critical.

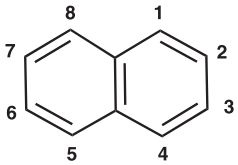
General Structure and Numbering System of Selected Aromatic Hydrocarbons



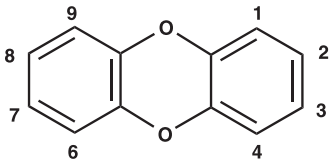
phenol



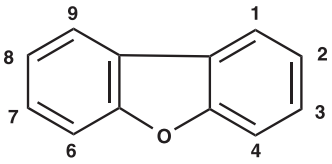
benzene



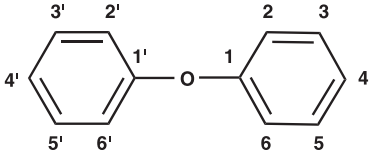
naphthalene



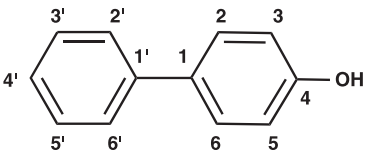
dibenzo-p-dioxin



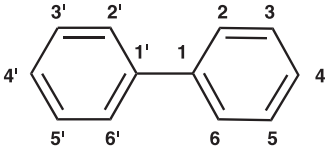
dibenzofuran



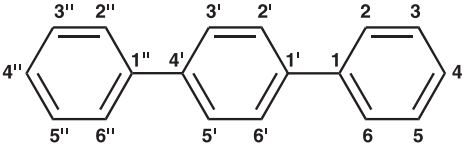
diphenyl ether



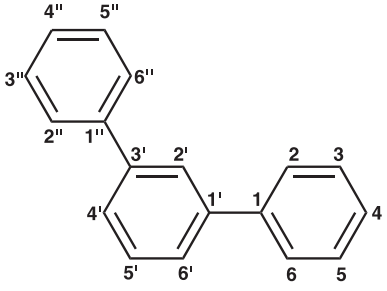
4-hydroxybiphenyl



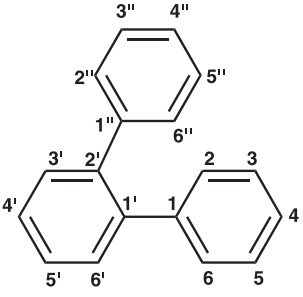
biphenyl



p-terphenyl



m-terphenyl



o-terphenyl

Number of Possible Isomers for Selected Halogenated Aromatic Compounds

# of X	Terphenyl			Biphenyl	Biphenylol	Dibenzo-p-dioxin	Dibenzofuran	Naphthalene	Benzene	Phenol
	ortho	meta	para							
1	5	6	4	3	19	2	4	2	1	3
2	28	28	21	12	64	10	16	10	3	6
3	80	87	55	24	136	14	28	14	3	6
4	211	211	139	42	198	22	38	22	3	3
5	355	382	226	46	198	14	28	14	1	1
6	544	544	351	42	136	10	16	10	1	
7	596	638	358	24	64	2	4	2		
8	544	544	351	12	19	1	1	1		
9	355	382	226	3	3					
10	211	211	139	1						
11	80	87	55							
12	28	28	21							
13	5	6	4							
14	1	1	1							

X= Halogen (does not apply to mixed halogenated compounds)
For diphenyl ethers use the biphenyl values

Molecular Weights for Selected Chlorinated and Brominated Aromatic Hydrocarbons

# of Cl/Br	PCTs	PCBs	PCDEs	PCDDs	PCDFs	PCNs	CBs	CPs	PBBs	PBDEs	PBDDs	PBDFs
0	230.31	154.21	170.21	184.19	168.19	128.17	78.11	94.11	154.21	170.21	184.19	168.19
1	264.75	188.66	204.66	218.64	202.64	162.62	112.56	128.56	233.11	249.11	263.09	247.09
2	299.20	223.10	239.10	253.08	237.09	197.06	147.00	163.00	312.00	328.00	341.99	325.99
3	333.64	257.55	273.55	287.53	271.53	231.51	181.45	197.45	390.90	406.90	420.88	404.88
4	368.09	291.99	307.99	321.97	305.98	265.95	215.89	231.89	469.80	485.80	499.78	483.78
5	402.53	326.44	342.44	356.42	340.42	300.40	250.34	266.34	548.69	564.69	578.67	562.68
6	436.98	360.88	376.88	390.86	374.87	334.84	284.78		627.59	643.59	657.57	641.57
7	471.42	395.33	411.33	425.31	409.31	369.29			706.48	722.48	736.47	720.47
8	505.87	429.77	445.77	459.75	443.76	403.73			785.38	801.38	815.36	799.36
9	540.31	464.22	480.22						864.28	880.28		
10	574.76	498.66	514.66						943.17	959.17		
11	609.20											
12	643.65											
13	678.09											
14	712.54											

Note: The molecular weight for PCHBs ($C_{12}H_{9-n}Cl_nOH$) is the same as the PCDEs ($C_{12}H_{10-n}Cl_nO$), but the maximum # of Chlorines is one less for the PCHBs.

PCTs = polychlorinated terphenyls, **PCBs** = polychlorinated biphenyls, **PCDEs** = polychlorinated diphenyl ethers
PCHBs = polychlorinated hydroxybiphenyls (biphenylols), **PCDDs** = polychlorinated dibenzo-p-dioxins,
PCDFs = polychlorinated dibenzofurans, **PCNs** = polychlorinated naphthalenes, **CBs** = chlorobenzenes, **CPs** = chlorophenols,
PBBs = polybrominated biphenyls, **PBDEs** = polybrominated diphenyl ethers,
PBDDs = polybrominated dibenzo-p-dioxins, **PBDFs** = polybrominated dibenzofurans

Exact Mass & Relative Ion Abundances of Selected Chlorinated Aromatic Hydrocarbons

	PCTs			PCBs			PCHBs			PCDDs		
	$^{12}C_{18}$	$C_{18}H_{14-n}Cl_n$	$^{13}C_{18}$	$^{12}C_{12}$	$C_{12}H_{10-n}Cl_n$	$^{13}C_{12}$	$^{12}C_{12}$	$C_{12}H_{9-n}Cl_nOH$	$^{13}C_{12}$	$^{12}C_{12}$	$C_{12}H_{8-n}Cl_nO_2$	$^{13}C_{12}$
# of Cl	Exact Mass	Relative Abundance	Exact Mass	Exact Mass	Relative Abundance	Exact Mass	Exact Mass	Relative Abundance	Exact Mass	Exact Mass	Relative Abundance	Exact Mass
0	230.1096	**100**	248.1699	154.0783	**100**	166.1185	170.0732	**100**	182.1134	184.0524	**100**	196.0927
1	264.0706	**100**	282.1310	188.0393	**100**	200.0795	204.0342	**100**	216.0745	218.0135	**100**	230.0537
	266.0676	34.4	284.1280	190.0363	33.2	202.0766	206.0312	33.5	218.0715	220.0105	33.7	232.0508
2	298.0316	**100**	316.0920	222.0003	**100**	234.0406	237.9952	**100**	250.0355	251.9745	**100**	264.0147
	300.0287	66.8	318.0890	223.9974	65.6	236.0376	239.9923	65.9	252.0325	253.9715	66.1	266.0118
	302.0257	11.8	320.0861	225.9944	11.0	238.0347	241.9893	11.2	254.0296	255.9686	11.3	268.0088
3	331.9926	**100**	350.0530	255.9613	**100**	268.0016	271.9562	**100**	283.9965	285.9355	**100**	297.9758
	333.9897	99.2	352.0501	257.9584	98.0	269.9986	273.9533	98.2	285.9936	287.9326	98.5	299.9728
	335.9867	33.4	354.0471	259.9554	32.3	271.9957	275.9503	32.5	287.9906	289.9296	32.7	301.9699
	337.9838	4.0	356.0442	261.9525	3.7	273.9927	277.9474	3.7	289.9877	291.9267	3.8	303.9669
4	365.9537	76.0	384.0141	289.9224	76.7	301.9626	305.9173	76.5	317.9575	319.8965	76.4	331.9368
	367.9507	**100**	386.0111	291.9194	**100**	303.9597	307.9143	**100**	319.9546	321.8936	**100**	333.9339
	369.9478	49.8	388.0082	293.9165	49.1	305.9567	309.9114	49.3	321.9516	323.8906	49.4	335.9309
	371.9448	11.3	390.0052	295.9135	10.8	307.9538	311.9084	10.9	323.9487	325.8877	11.0	337.9280
5	399.9147	61.0	417.9751	323.8834	61.4	335.9237	339.8783	61.3	351.9186	353.8576	61.3	365.8978
	401.9117	**100**	419.9721	325.8804	**100**	337.9207	341.8754	**100**	353.9156	355.8546	**100**	367.8949
	403.9088	66.0	421.9692	327.8775	65.3	339.9178	343.8724	65.4	355.9127	357.8517	65.5	369.8919
	405.9058	22.0	423.9662	329.8745	21.4	341.9148	345.8695	21.5	357.9097	359.8487	21.6	371.8890
6	433.8757	50.9	451.9361	357.8444	51.2	369.8847	373.8393	51.2	385.8796	387.8186	51.1	399.8589
	435.8728	**100**	453.9332	359.8415	**100**	371.8817	375.8364	**100**	387.8766	389.8156	**100**	401.8559
	437.8698	82.1	455.9302	361.8385	81.5	373.8788	377.8334	81.6	389.8737	391.8127	81.7	403.8530
	439.8669	36.2	457.9273	363.8356	35.5	375.8758	379.8305	35.6	391.8707	393.8097	35.8	405.8500
7	467.8367	43.7	485.8971	391.8054	43.9	403.8457	407.8004	43.9	419.8406	421.7796	43.9	433.8199
	469.8338	**100**	487.8942	393.8025	**100**	405.8428	409.7974	**100**	421.8377	423.7767	**100**	435.8169
	471.8308	98.3	489.8912	395.7995	97.7	407.8398	411.7945	97.8	423.8347	425.7737	97.9	437.8140
	473.8279	53.9	491.8883	397.7966	53.1	409.8369	413.7915	53.3	425.8318	427.7708	53.4	439.8110
	475.8249	17.9	493.8853	399.7936	17.4	411.8339	415.7886	17.5	427.8288	429.7678	17.6	441.8081
8	501.7978	33.5	519.8582	425.7665	33.8	437.8067	441.7614	33.7	453.8016	455.7407	33.7	467.7809
	503.7948	87.4	521.8552	427.7635	87.8	439.8038	443.7584	87.7	455.7987	457.7377	87.6	469.7780
	505.7919	**100**	523.8523	429.7606	**100**	441.8008	445.7555	**100**	457.7957	459.7348	**100**	471.7750
	507.7889	65.6	525.8493	431.7576	65.2	443.7979	447.7525	65.2	459.7928	461.7318	65.3	473.7721
	509.7860	27.0	527.8464	433.7547	26.6	445.7949	449.7496	26.7	461.7898	463.7289	26.8	475.7691
9	535.7588	26.1	553.8192	459.7275	26.3	471.7678	475.7224	26.3	487.7627			
	537.7559	76.5	555.8162	461.7246	76.9	473.7648	477.7195	76.8	489.7597			
	539.7529	**100**	557.8133	463.7216	**100**	475.7619	479.7165	**100**	491.7568			
	541.7500	76.4	559.8103	465.7187	75.9	477.7589	481.7136	76.0	493.7538			
	543.7470	37.6	561.8074	467.7157	37.1	479.7560	483.7106	37.2	495.7509			
10	569.7198	20.9	587.7802	493.6885	21.1	505.7288						
	571.7169	68.1	589.7773	495.6856	68.4	507.7258						
	573.7139	**100**	591.7743	497.6826	**100**	509.7229						
	575.7110	87.2	593.7714	499.6797	86.7	511.7199						
	577.7080	50.0	595.7684	501.6767	49.4	513.7170						
11	603.6809	17.1	621.7412									
	605.6779	61.3	623.7383									
	607.6750	**100**	625.7353									
	609.6720	98.0	627.7324									
	611.6691	64.1	629.7294									
	613.6661	29.4	631.7265									
12	637.6419	13.1	655.7023									
	639.6389	51.3	657.6993									
	641.6360	92.0	659.6964									
	643.6330	**100**	661.6934									
	645.6301	73.5	663.6905									
	647.6271	38.5	665.6875									
13	671.6029	10.1	689.6633									
	673.6000	42.8	691.6604									
	675.5970	83.7	693.6574									
	677.5941	**100**	695.6545									
	679.5911	81.6	697.6515									
	681.5882	48.0	699.6486									
14	705.5639	8.0	723.6243									
	707.5610	36.3	725.6214									
	709.5580	76.7	727.6184									
	711.5551	**100**	729.6155									
	713.5521	89.7	731.6125									
	715.5492	58.6	733.6096									

Exact Mass & Relative Ion Abundances of Selected Chlorinated Aromatic Hydrocarbons

	PCDFs			PCNs			CBs			CPs		
	$^{12}C_{12}$	$C_{12}H_{8-n}Cl_nO$	$^{13}C_{12}$	$^{12}C_{10}$	$C_{10}H_{8-n}Cl_n$	$^{13}C_{10}$	$^{12}C_6$	$C_6H_{6-n}Cl_n$	$^{13}C_6$	$^{12}C_6$	$C_6H_{5-n}Cl_nOH$	$^{13}C_6$
# of Cl	Exact Mass	Relative Abundance	Exact Mass	Exact Mass	Relative Abundance	Exact Mass	Exact Mass	Relative Abundance	Exact Mass	Exact Mass	Relative Abundance	Exact Mass
0	168.0575	**100**	180.0978	128.0626	**100**	138.0962	78.0470	**100**	84.0671	94.0419	**100**	100.0620
1	202.0185	**100**	214.0588	162.0236	**100**	172.0572	112.0080	**100**	118.0281	128.0029	**100**	134.0230
	204.0156	33.5	216.0559	164.0207	33.0	174.0542	114.0050	32.6	120.0252	129.9999	32.8	136.0201
2	235.9796	**100**	248.0198	195.9847	**100**	206.0182	145.9690	**100**	151.9891	161.9639	**100**	167.9841
	237.9766	65.8	250.0169	197.9817	65.4	208.0153	147.9661	65.0	153.9862	163.9610	65.2	169.9811
	239.9737	11.2	252.0139	199.9788	10.9	210.0123	149.9631	10.6	155.9832	165.9580	10.8	171.9782
3	269.9406	**100**	281.9809	229.9457	**100**	239.9792	179.9300	**100**	185.9502	195.9249	**100**	201.9451
	271.9376	98.2	283.9779	231.9427	97.8	241.9763	181.9271	97.4	187.9472	197.9220	97.6	203.9421
	273.9347	32.5	285.9750	233.9398	32.0	243.9733	183.9241	31.7	189.9443	199.9190	31.9	205.9392
	275.9317	3.7	287.9720	235.9368	3.6	245.9704	185.9212	3.5	191.9413	201.9161	3.5	207.9362
4	303.9016	76.5	315.9419	263.9067	76.8	273.9403	213.8911	77.1	219.9112	229.8860	76.9	235.9061
	305.8987	**100**	317.9389	265.9038	**100**	275.9373	215.8881	**100**	221.9082	231.8830	**100**	237.9032
	307.8957	49.2	319.9360	267.9008	49.0	277.9344	217.8852	48.7	223.9053	233.8801	48.8	239.9002
	309.8928	10.9	321.9330	269.8979	10.7	279.9314	219.8822	10.6	225.9023	235.8771	10.7	241.8973
5	337.8627	61.3	349.9029	297.8677	61.5	307.9013	247.8521	61.7	253.8722	263.8470	61.6	269.8671
	339.8597	**100**	351.9000	299.8648	**100**	309.8983	249.8491	**100**	255.8693	265.8441	**100**	271.8642
	341.8568	65.4	353.8970	301.8618	65.1	311.8954	251.8462	64.9	257.8663	267.8411	65.0	273.8612
	343.8538	21.5	355.8941	303.8589	21.3	313.8924	253.8432	21.1	259.8634	269.8382	21.2	275.8583
6	371.8237	51.2	383.8639	331.8288	51.3	341.8623	281.8131	51.4	287.8332			
	373.8207	**100**	385.8610	333.8258	**100**	343.8594	283.8102	**100**	289.8303			
	375.8178	81.6	387.8580	335.8229	81.3	345.8564	285.8072	81.1	291.8273			
	377.8148	35.6	389.8551	337.8199	35.3	347.8535	287.8043	35.1	293.8244			
7	405.7847	43.9	417.8250	365.7898	44.0	375.8233						
	407.7818	**100**	419.8220	367.7868	**100**	377.8204						
	409.7788	97.8	421.8191	369.7839	97.5	379.8174						
	411.7759	53.3	423.8161	371.7809	52.9	381.8145						
	413.7729	17.5	425.8132	373.7780	17.3	383.8115						
8	439.7457	33.7	451.7860	399.7508	33.9	409.7844						
	441.7428	87.7	453.7830	401.7479	87.9	411.7814						
	443.7398	**100**	455.7801	403.7449	**100**	413.7785						
	445.7369	65.2	457.7771	405.7420	65.0	415.7755						
	447.7339	26.7	459.7742	407.7390	26.5	417.7726						

PCTs = polychlorinated terphenyls
PCBs = polychlorinated biphenyls
PCHBs = polychlorinated hydroxybiphenyls
PCDDs = polychlorinated dibenzo-p-dioxins
PCDFs = polychlorinated dibenzofurans
PCNs = polychlorinated naphthalenes
CBs = chlorobenzenes
CPs = chlorophenols

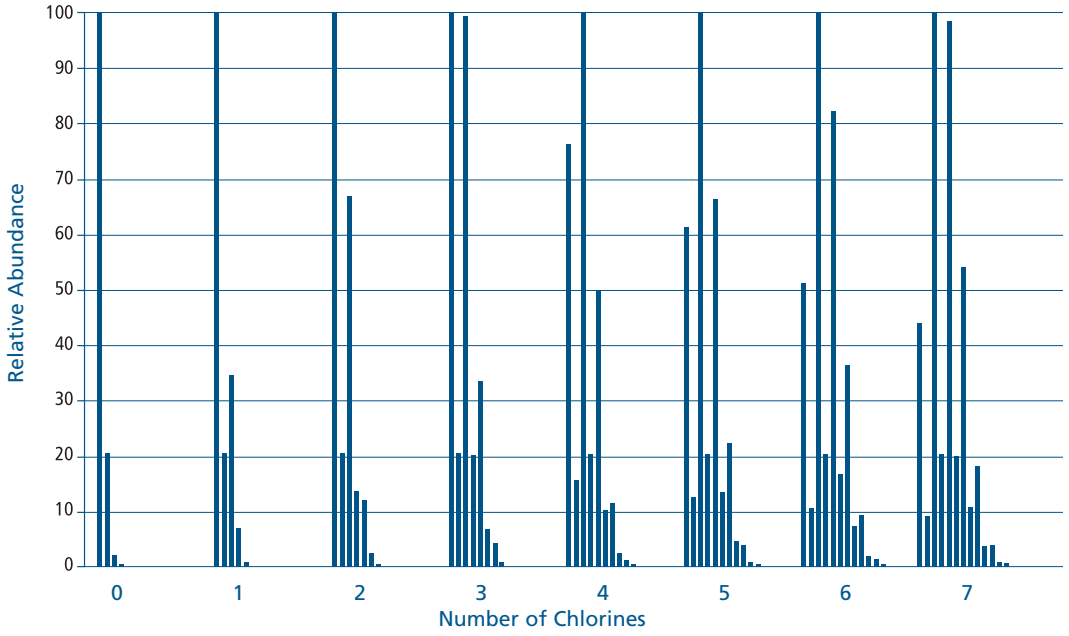
Accurate masses: ^{12}C=12.000000, ^{13}C=13.003355, ^{1}H=1.007825, ^{35}Cl= 34.968853, ^{37}Cl=36.965903, ^{16}O=15.994915

Relative abundances of isotopes were determined using the method described in: Pretsch,Clerc,Seibl,Simon,
Tables of Spectral Data for Structure Determination of Organic Compounds, Springer-Verlag, 1983.
The following natural isotopic abundances were used in all calculations: ^{12}C=98.89%, ^{13}C=1.11%, ^{1}H=99.985%, ^{2}H=0.015%, ^{35}Cl=75.53%, ^{37}Cl=24.47%, ^{16}O=99.759%, ^{17}O=0.037%, ^{18}O=0.204%.

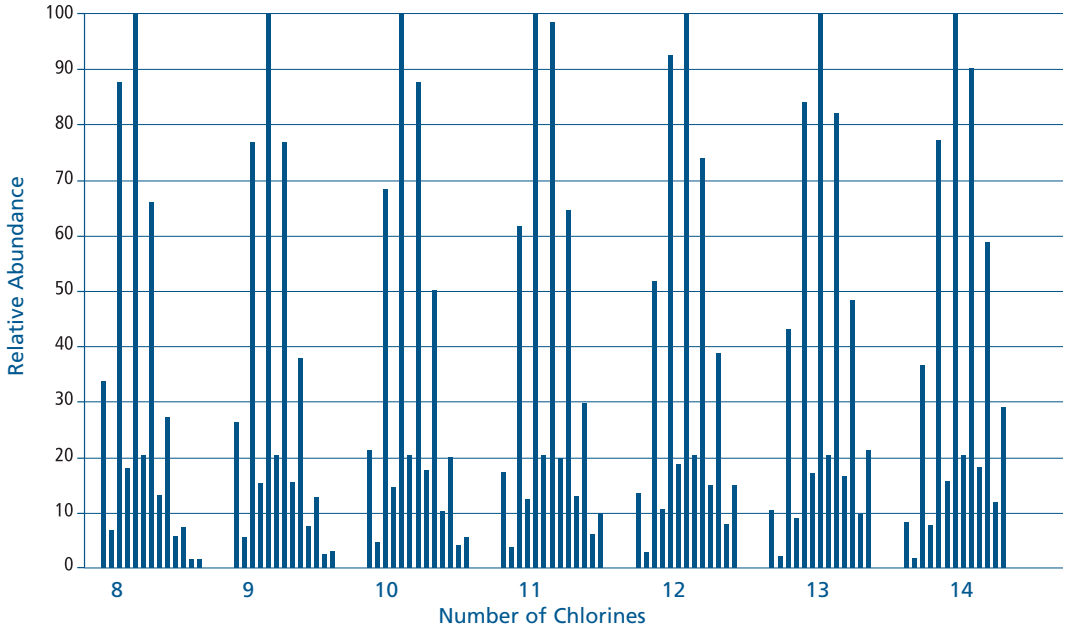
Cl_n

MOLECULAR ION CLUSTERS FOR CHLORINATED AROMATIC COMPOUNDS

Molecular Ion Cluster



Molecular Ion Cluster

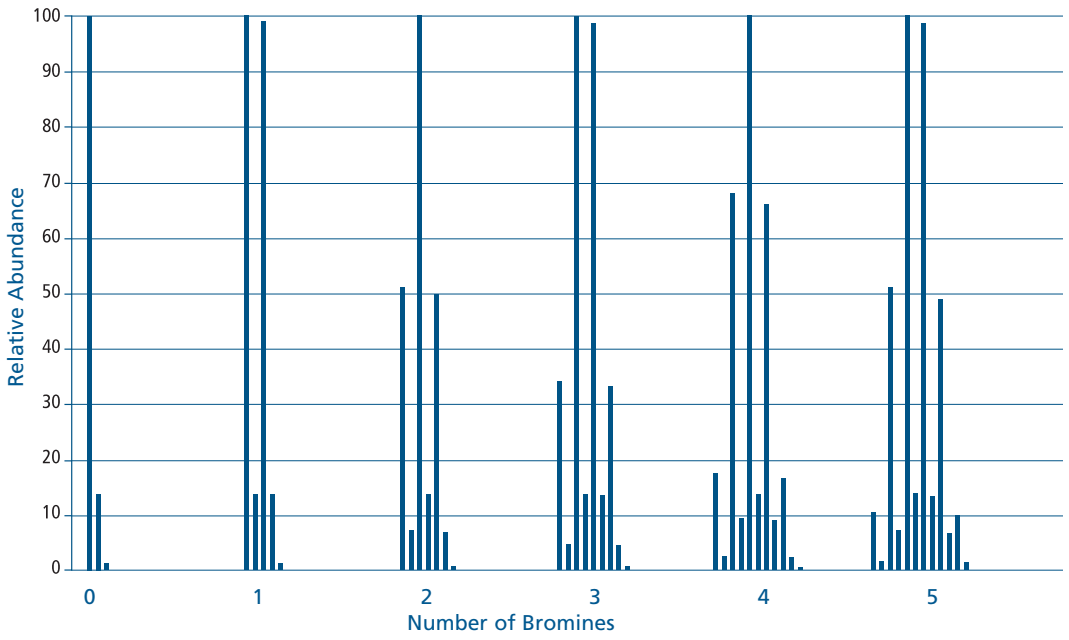


Ions shown are M, M+1, M+2, M+3, M+4, M+5, M+6, M+7, M+8, M+9, M+10, M+11, M+12, and are representative of chlorinated terphenyls ($C_{18}H_{14-n}Cl_n$)

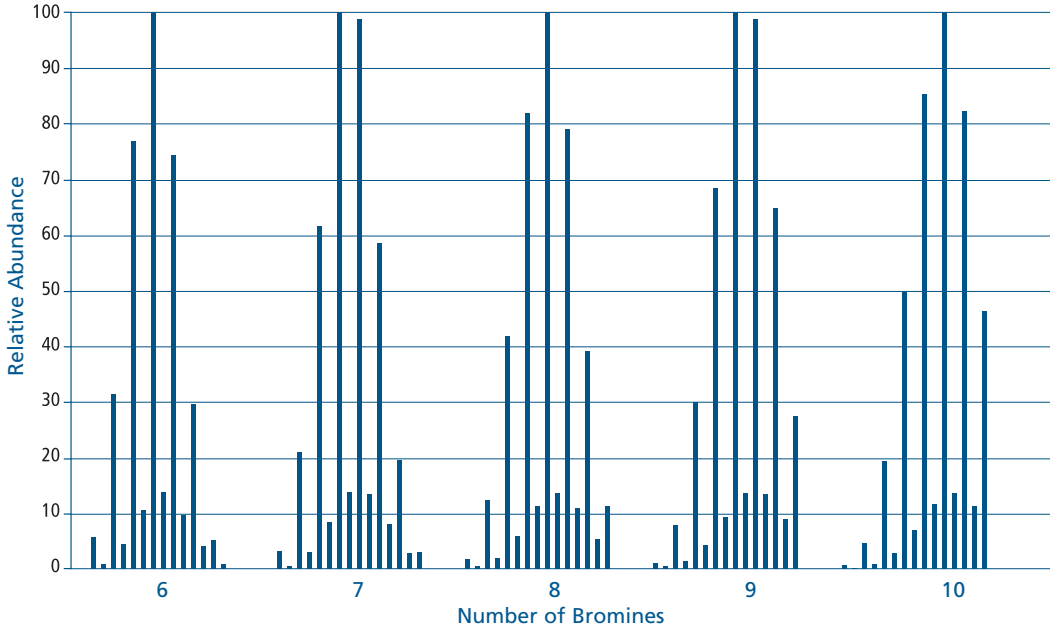
MOLECULAR ION CLUSTERS FOR BROMINATED AROMATIC COMPOUNDS

Br_n

Molecular Ion Cluster



Molecular Ion Cluster



Ions shown are M, M+1, M+2, M+3, M+4, M+5, M+6, M+7, M+8, M+9, M+10, M+11, M+12, M+13, M+14 and are representative of brominated diphenyl ethers ($C_{12}H_{10-n}Br_nO$)

Exact Mass & Relative Ion Abundances of Selected Brominated Aromatic Hydrocarbons

	PBBs			PBDEs			PBDDs			PBDFs		
	$^{12}C_{12}$	$C_{12}H_{10-n}Br_n$	$^{13}C_{12}$	$^{12}C_{12}$	$C_{12}H_{10-n}Br_nO$	$^{13}C_{12}$	$^{12}C_{12}$	$C_{12}H_{8-n}Br_nO_2$	$^{13}C_{12}$	$^{12}C_{12}$	$C_{12}H_{8-n}Br_nO$	$^{13}C_{12}$
# of Br	Exact Mass	Relative Abundance	Exact Mass	Exact Mass	Relative Abundance	Exact Mass	Exact Mass	Relative Abundance	Exact Mass	Exact Mass	Relative Abundance	Exact Mass
0	154.0783	**100**	166.1185	170.0732	**100**	182.1134	184.0524	**100**	196.0927	168.0575	**100**	180.0978
1	231.9887	**100**	244.0290	247.9836	**100**	260.0239	261.9629	**100**	274.0032	245.9680	**100**	258.0083
	233.9867	98.7	246.0270	249.9816	98.9	262.0219	263.9609	99.1	276.0012	247.9660	98.9	260.0063
2	309.8992	50.9	321.9395	325.8941	50.8	337.9344	339.8734	50.8	351.9136	323.8785	50.8	335.9187
	311.8972	**100**	323.9375	327.8921	**100**	339.9324	341.8714	**100**	353.9116	325.8765	**100**	337.9167
	313.8952	49.6	325.9355	329.8901	49.7	341.9304	343.8694	49.9	355.9096	327.8745	49.7	339.9147
3	387.8097	34.0	399.8499	403.8046	33.9	415.8449	417.7839	33.9	429.8241	401.7889	33.9	413.8292
	389.8077	**100**	401.8479	405.8026	**100**	417.8429	419.7819	**100**	431.8221	403.7869	**100**	415.8272
	391.8057	98.4	403.8459	407.8006	98.6	419.8409	421.7799	98.7	433.8201	405.7849	98.6	417.8252
	393.8037	32.7	405.8439	409.7986	32.8	421.8389	423.7779	33.0	435.8181	407.7829	32.8	419.8232
4	465.7202	17.3	477.7604	481.7151	17.3	493.7553	495.6943	17.3	507.7346	479.6994	17.3	491.7397
	467.7182	67.9	479.7584	483.7131	67.8	495.7533	497.6923	67.8	509.7326	481.6974	67.8	493.7377
	469.7162	**100**	481.7564	485.7111	**100**	497.7513	499.6903	**100**	511.7306	483.6954	**100**	495.7357
	471.7142	65.7	483.7544	487.7091	65.8	499.7493	501.6883	65.9	513.7286	485.6934	65.8	497.7337
	473.7122	16.4	485.7524	489.7071	16.5	501.7473	503.6863	16.6	515.7266	487.6914	16.5	499.7317
5	543.6306	10.4	555.6709	559.6255	10.4	571.6658	573.6048	10.4	585.6451	557.6099	10.4	569.6502
	545.6286	51.0	557.6689	561.6235	50.9	573.6638	575.6028	50.9	587.6431	559.6079	50.9	571.6482
	547.6266	**100**	559.6669	563.6215	**100**	575.6618	577.6008	**100**	589.6411	561.6059	**100**	573.6462
	549.6246	98.3	561.6649	565.6195	98.4	577.6598	579.5988	98.5	591.6391	563.6039	98.4	575.6442
	551.6226	48.5	563.6629	567.6175	48.7	579.6578	581.5968	48.8	593.6371	565.6019	48.7	577.6422
	553.6206	9.7	565.6609	569.6155	9.8	581.6558	583.5948	9.9	595.6351	567.5999	9.8	579.6402
6	621.5411	5.3	633.5814	637.5360	5.3	649.5763	651.5153	5.3	663.5555	635.5204	5.3	647.5606
	623.5391	31.2	635.5794	639.5340	31.1	651.5743	653.5133	31.1	665.5535	637.5184	31.1	649.5586
	625.5371	76.4	637.5774	641.5320	76.4	653.5723	655.5113	76.3	667.5515	639.5164	76.4	651.5566
	627.5351	**100**	639.5754	643.5300	**100**	655.5703	657.5093	**100**	669.5495	641.5144	**100**	653.5546
	629.5331	73.8	641.5734	645.5280	73.9	657.5683	659.5073	73.9	671.5475	643.5124	73.9	655.5526
	631.5311	29.2	643.5714	647.5260	29.3	659.5663	661.5053	29.4	673.5455	645.5104	29.3	657.5506
7	699.4516	3.0	711.4918	715.4465	3.0	727.4868	729.4258	3.0	741.4660	713.4308	3.0	725.4711
	701.4496	20.8	713.4898	717.4445	20.8	729.4848	731.4238	20.8	743.4640	715.4288	20.8	727.4691
	703.4476	61.2	715.4878	719.4425	61.1	731.4828	733.4218	61.1	745.4620	717.4268	61.1	729.4671
	705.4456	**100**	717.4858	721.4405	**100**	733.4808	735.4198	**100**	747.4600	719.4248	**100**	731.4651
	707.4436	98.2	719.4838	723.4385	98.3	735.4788	737.4178	98.4	749.4580	721.4228	98.3	733.4631
	709.4416	58.0	721.4818	725.4365	58.1	737.4768	739.4158	58.2	751.4560	723.4208	58.1	735.4611
8	777.3621	1.5	789.4023	793.3570	1.5	805.3972	807.3362	1.5	819.3765	791.3413	1.5	803.3816
	779.3601	12.1	791.4003	795.3550	12.1	807.3952	809.3342	12.1	821.3745	793.3393	12.1	805.3796
	781.3581	41.6	793.3983	797.3530	41.5	809.3932	811.3322	41.5	823.3725	795.3373	41.5	807.3776
	783.3561	81.5	795.3963	799.3510	81.5	811.3912	813.3302	81.4	825.3705	797.3353	81.5	809.3756
	785.3541	**100**	797.3943	801.3490	**100**	813.3892	815.3282	**100**	827.3685	799.3333	**100**	811.3736
	787.3521	78.6	799.3923	803.3470	78.7	815.3872	817.3262	78.7	829.3665	801.3313	78.7	813.3716
	789.3501	38.7	801.3903	805.3450	38.8	817.3852	819.3242	38.9	831.3645	803.3293	38.8	815.3696
9	855.2725	0.9	867.3128	871.2674	0.9	883.3077						
	857.2705	7.6	869.3108	873.2654	7.6	885.3057						
	859.2685	29.7	871.3088	875.2634	29.7	887.3037						
	861.2665	68.0	873.3068	877.2614	68.0	889.3017						
	863.2645	**100**	875.3048	879.2594	**100**	891.2997						
	865.2625	98.1	877.3028	881.2574	98.2	893.2977						
	867.2605	64.3	879.3008	883.2554	64.4	895.2957						
	869.2585	27.2	881.2988	885.2534	27.3	897.2937						
10	933.1830	0.4	945.2233	949.1779	0.4	961.2182						
	935.1810	4.3	947.2213	951.1759	4.3	963.2162						
	937.1790	19.0	949.2193	953.1739	18.9	965.2142						
	939.1770	49.5	951.2173	955.1719	49.5	967.2122						
	941.1750	85.0	953.2153	957.1699	84.9	969.2102						
	943.1730	**100**	955.2133	959.1679	**100**	971.2082						
	945.1710	81.8	957.2113	961.1659	81.9	973.2062						
	947.1690	46.0	959.2093	963.1639	46.0	975.2042						
	949.1670	17.0	961.2073	965.1619	17.1	977.2022						

PBBs = polybrominated biphenyls
PBDEs = polybrominated diphenyl ethers
PBDDs = polybrominated dibenzo-p-dioxins
PBDFs = polybrominated dibenzofurans

Accurate masses: ^{12}C=12.000000 , ^{13}C = 13.003355, ^{1}H=1.007825, ^{79}Br=78.918300, ^{81}Br= 80.916300, ^{16}O=15.994915

Relative abundances of isotopes were determined using the method described in: Pretsch,Clerc,Seibl,Simon, Tables of Spectral Data for Structure Determination of Organic Compounds, Springer-Verlag, 1983.
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Conversion Factors and Units of Measure

Prefix	Symbol	Factor	Fraction	
centi	c	10^{-2}	= 1/100	part per hundred
milli	m	10^{-3}	= 1/1,000	part per thousand
micro	µ	10^{-6}	= 1/1,000,000	part per million (ppm)
nano	n	10^{-9}	= 1/1,000,000,000	part per billion (ppb)
pico	p	10^{-12}	= 1/1,000,000,000,000	part per trillion (ppt)
femto	f	10^{-15}	= 1/1,000,000,000,000,000	part per quadrillion (ppq)
atto	a	10^{-18}	= 1/1,000,000,000,000,000,000	part per quintillion
zepto	z	10^{-21}	= 1/1,000,000,000,000,000,000,000	part per sextillion
yocto	y	10^{-24}	= 1/1,000,000,000,000,000,000,000,000	part per septillion

Commonly Used Units of Measure

wt/wt basis				wt/vol basis			
ppm	mg/kg	µg/g	ng/mg	**ppm**	mg/l	µg/ml	ng/µl
ppb	µg/kg	ng/g	pg/mg	**ppb**	µg/l	ng/ml	pg/µl
ppt	ng/kg	pg/g	fg/mg	**ppt**	ng/l	pg/ml	fg/µl
ppq	pg/kg	fg/g	ag/mg	**ppq**	pg/l	fg/ml	ag/µl

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Although a few items have been updated, this is essentially the fourth printing of the second edition of our reference guide. As always, we continue to expand our inventory of compounds of potential environmental and/or toxicological concern. Rather than trying to include these emerging contaminants in this guide, we will prepare and post separate reference guides, specific to these new standards, on our website.

As before, if you have any comments or suggestions for future reference guides or if you would like to receive additional copies of this guide, please contact us at:

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