

GLOBAL ANALYTICAL SOLUTIONS



GERSTEL

TechNote 1/2000

Volatile Organic Compounds in Air

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SYSTEM

Thermodesorption System TDS 2
with Autosampler TDS A
Cooled Injection System CIS 4
Gas Chromatograph Agilent 6890
Mass Selective Detector Agilent 5973

SUMMARY

System performance of the GERSTEL TDS A in conjunction with an Agilent GC-MSD system was tested using a 43 component gas calibration mixture which was developed for the Japanese Hazardous Air Pollutants (JHAP) monitoring method. A five-point calibration curve was obtained for each compound (2-20 ppb@1L) with an average correlation coefficient of 0.996. Twelve replicate analyses of the mixture, where each component was present at 20 ppb@1L, gave an average percent relative standard deviation (%RSD) of 4.6.

SAMPLE PREPARATION

Samples were prepared by injecting different volumes of a 1000 ppb JHAPS-43 gas calibration mix (SUPELCO 500429) onto Carbotrap 300 TDS tubes (GERSTEL GI 8273-U). Complete transfer of the analytes was obtained by injecting the calibration mix into a 50 mL/min helium stream heated to 65°C, and allowing a total of 200 mL of gas to pass through the adsorbent bed.

Table 1 provides all information relating to the calibration mixture and sample preparation.

	R.T.	2 ppb@1L	5 ppb@1L	10 ppb@1L	15 ppb@1L	20 ppb@1L	Slope	Intercept	Corr
Halocarbon 12	5,0	148214	320312	612024	770947	1191553	55187	34670	0,991
Chloromethane	5,6	11415	25159	55479	69886	115500	5518	-1895	0,986
Halocarbon 114	6,0	186526	467386	807162	1318451	1929355	94621	-42278	0,994
Vinyl Chloride	6,4	53180	108005	241498	267728	488608	22494	-2130	0,970
1,3-Butadiene	7,0	42944	108718	216839	318452	432614	21498	331	1,000
Bromomethane	7,9	45347	69490	171526	198322	400003	18422	-14650	0,956
Ethyl Chloride	8,6	10179	21333	41849	59694	93945	4498	-1382	0,991
Halocarbon 11	11,2	183185	446414	887688	1313537	1849206	91417	-14735	0,999
Acrylonitrile	11,9	30182	78116	153648	254261	331895	16975	-6915	0,999
1,1-Dichloroethylene	13,0	91429	229965	465081	688485	937522	46770	-3913	1,000
Methylene Chloride	13,2	64978	158991	295621	421656	616801	29729	2424	0,997
3-Chloropropylene	13,6	30192	74367	152486	248506	321021	16458	-5844	0,999
Halocarbon 113	14,0	178311	431661	876366	1391207	1768082	90027	-7158	0,999
1,1 Dichloroethane	16,1	116934	284651	577776	917519	1173006	59714	-7046	0,999
cis-1,2 Dichloroethane	17,9	82224	207584	411853	651941	840105	42625	-4554	0,999
Chloroform	18,5	143381	355500	726476	1161585	1501682	76664	-19580	0,999
1,2 Dichloroethane	20,0	78306	199972	370906	626286	788013	40149	-4857	0,998
1,1,1 Trichloroethane	20,6	155978	386504	764089	1280960	1609959	82763	-21236	0,998
Benzene	21,5	251788	616971	1208228	1881052	2473110	124131	-4733	1,000
Carbon Tetrachloride	21,8	176407	429943	857377	1440967	1864290	95587	-40309	0,998
1,2-Dichloropropane	22,8	74951	179809	369311	596225	778034	39697	-13187	0,999
Trichloroethylene	23,2	119805	301714	585421	940635	1203847	61042	-4548	0,999
cis-1,3 Dichloropropene	24,3	121959	270995	552355	970396	1282772	65993	-46630	0,997
trans-1,3-Dichloropropene	25,0	100884	223696	418368	757227	1009031	51347	-32169	0,995
1,1,2-Trichloroethane	25,3	106992	245551	501896	819413	1094652	55593	-24470	0,999
Toluene	25,6	364498	779802	1594336	2432866	3214434	160128	11855	1,000
1,2-Dibromoethane	26,5	159459	355381	739327	1213374	1640499	83377	-45517	0,998
Tetrachloroethylene	27,0	198701	432841	930177	1447907	1953423	98662	-33475	0,999
Chlorobenzene	27,7	302860	673802	1362475	2130443	2856142	143018	-22244	1,000
Ethylbenzene	28,1	447638	1007621	2026586	3169419	4251350	212853	-33152	1,000
m,p-Xylene	28,3	676166	1606864	3137393	4920259	6523747	326685	-24643	1,000
Styrene	28,6	241303	582499	1147369	1841611	2505372	126133	-48154	0,999
1,1,2,2-Tetrachlorethylene	28,8	201975	474906	953891	1498491	2056534	103157	-35677	0,999
o-xylene	28,8	351457	841913	1628705	2565469	3424778	171337	-19437	1,000
4-Ethyltoluene	30,0	429271	961482	2135392	3124711	4216006	211985	-31276	1,000
1,3,5-Trimethylbenzene	30,1	410775	1035009	2102407	2973397	4031829	199356	37383	0,999
1,2,4-Trimethylbenzene	30,6	415871	945283	2030568	2979086	4108119	205120	-37467	0,999
1,3-Dichlorobenzene	30,9	331826	779357	1591570	2534901	3442843	173918	-72649	0,999
1,4-Dichlorobenzene	31,0	331272	791003	1623149	2526463	3378196	170493	-43108	1,000
1,2-Dichlorobenzene	31,4	307090	735363	1493570	2355003	3190170	160932	-57454	0,999
1,2,4-Trichlorobenzene	34,2	288266	729459	1283242	2222498	3166380	158288	-108223	0,995
Hexachloro-1,3-butadiene	35,1	257850	740682	1170465	1948798	2692014	132148	-12379	0,996

Table 1. Analyte Data for Calibration Mix.

ANALYSIS

TDS tubes were analyzed using the GERSTEL TDS A ThermoDesorption System in conjunction with an Agilent 5973 MSD. The Gerstel system was operated in the TDS splitless/ CIS split mode and the MSD was operated in the EI full scan mode.

THERMODESORPTION SYSTEM TDS 2

Tube type	Carbotrap 300
Pneumatics mode	splitless
Sample mode	sample remove
Initial temperature	25°C (1 min)
Ramp	60°C/min
Final temperature	330°C (1 min)
Transferline temp.	275°C

MASS SELECTIVE DETECTOR 5973

Scan mode	
Tune	Atune
EM Offset	none
Mass range	35-269 amu
Threshold	200
Scans/sec	3.13
Transferline temp.	280°C
Source temperature	230°C
Quad temperature	150°C

COOLED INJECTION SYSTEM CIS 4

Liquid nitrogen option

Liner type	Carbotrap C/Glassbeads
Carrier gas	Helium
Pneumatics mode	solvent venting
Vent pressure	26.9 psi
Vent flow	20 ml/min
Vent time	until 0.00 min
Split Flow	10 ml/min @ 0.01 min
Initial temperature	-150°C (0.1 min)
Ramp	12°C/sec
Final temperature	350°C (3 min)

GAS CHROMATOGRAPH 6890

Column	SPB-1 (Supelco) 60 m, 0.25 mm, 3.0 µm
Mode	constant flow, 1.5 ml/min
Initial temperature	35°C (8 min)
Ramp 1	5°C/min
Final temperature 1	100°C
Ramp 2	15°C/min
Final temperature 2	230°C (8 min)

RESULTS

Figure 1 shows the chromatogram of the analytes present at 5 ppb@1L. This figure shows the excellent peak shape obtained for the entire range of compounds.

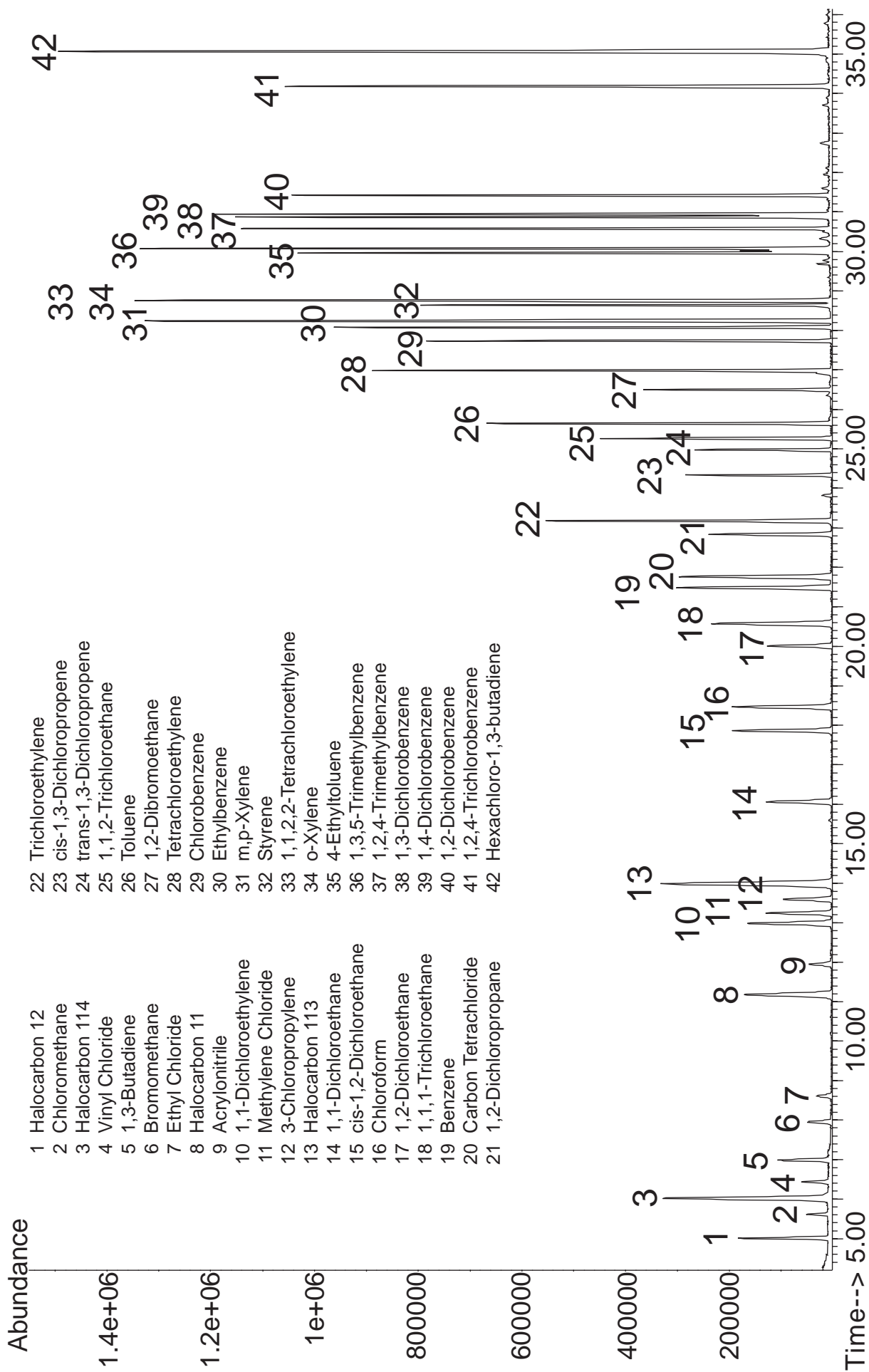


Figure 1. Chromatogram of analytes at 5ppb@1L.

Table 2 shows the data obtained for a five-point calibration curve of the analytes present at 2, 5, 10, 15 and 20 ppb@1L.

		2 ppb@1L	5 ppb@1L	10 ppb@1L	15 ppb@1L	20 ppb@1L			
	R.T.	2	5	10	15	20	Slope	Intercept	Corr
Halocarbon 12	5,0	148214	320312	612024	770947	1191553	55187	34670	0,991
Chloromethane	5,6	11415	25159	55479	69886	115500	5518	-1895	0,986
Halocarbon 114	6,0	186526	467386	807162	1318451	1929355	94621	-42278	0,994
Vinyl Chloride	6,4	53180	108005	241498	267728	488608	22494	-2130	0,970
1,3-Butadiene	7,0	42944	108718	216839	318452	432614	21498	331	1,000
Bromomethane	7,9	45347	69490	171526	198322	400003	18422	-14650	0,956
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Halocarbon 11	11,2	183185	446414	887688	1313537	1849206	91417	-14735	0,999
Acrylonitrile	11,9	30182	78116	153648	254261	331895	16975	-6915	0,999
1,1-Dichloroethylene	13,0	91429	229965	465081	688485	937522	46770	-3913	1,000
Methylene Chloride	13,2	64978	158991	295621	421656	616801	29729	2424	0,997
3-Chloropropylene	13,6	30192	74367	152486	248506	321021	16458	-5844	0,999
Halocarbon 113	14,0	178311	431661	876366	1391207	1768082	90027	-7158	0,999
1,1 Dichloroethane	16,1	116934	284651	577776	917519	1173006	59714	-7046	0,999
cis-1,2 Dichloroethane	17,9	82224	207584	411853	651941	840105	42625	-4554	0,999
Chloroform	18,5	143381	355500	726476	1161585	1501682	76664	-19580	0,999
1,2 Dichloroethane	20,0	78306	199972	370906	626286	788013	40149	-4857	0,998
1,1,1 Trichloroethane	20,6	155978	386504	764089	1280960	1609959	82763	-21236	0,998
Benzene	21,5	251788	616971	1208228	1881052	2473110	124131	-4733	1,000
Carbon Tetrachloride	21,8	176407	429943	857377	1440967	1864290	95587	-40309	0,998
1,2-Dichloropropane	22,8	74951	179809	369311	596225	778034	39697	-13187	0,999
Trichloroethylene	23,2	119805	301714	585421	940635	1203847	61042	-4548	0,999
cis-1,3 Dichloropropene	24,3	121959	270995	552355	970396	1282772	65993	-46630	0,997
trans-1,3-Dichloropropene	25,0	100884	223696	418368	757227	1009031	51347	-32169	0,995
1,1,2-Trichloroethane	25,3	106992	245551	501896	819413	1094652	55593	-24470	0,999
Toluene	25,6	364498	779802	1594336	2432866	3214434	160128	11855	1,000
1,2-Dibromoethane	26,5	159459	355381	739327	1213374	1640499	83377	-45517	0,998
Tetrachloroethylene	27,0	198701	432841	930177	1447907	1953423	98662	-33475	0,999
Chlorobenzene	27,7	302860	673802	1362475	2130443	2856142	143018	-22244	1,000
Ethylbenzene	28,1	447638	1007621	2026586	3169419	4251350	212853	-33152	1,000
m,p-Xylene	28,3	676166	1606864	3137393	4920259	6523747	326685	-24643	1,000
Styrene	28,6	241303	582499	1147369	1841611	2505372	126133	-48154	0,999
1,1,2,2-Tetrachlorethylene	28,8	201975	474906	953891	1498491	2056534	103157	-35677	0,999
o-xylene	28,8	351457	841913	1628705	2565469	3424778	171337	-19437	1,000
4-Ethyltoluene	30,0	429271	961482	2135392	3124711	4216006	211985	-31276	1,000
1,3,5-Trimethylbenzene	30,1	410775	1035009	2102407	2973397	4031829	199356	37383	0,999
1,2,4-Trimethylbenzene	30,6	415871	945283	2030568	2979086	4108119	205120	-37467	0,999
1,3-Dichlorobenzene	30,9	331826	779357	1591570	2534901	3442843	173918	-72649	0,999
1,4-Dichlorobenzene	31,0	331272	791003	1623149	2526463	3378196	170493	-43108	1,000
1,2-Dichlorobenzene	31,4	307090	735363	1493570	2355003	3190170	160932	-57454	0,999
1,2,4-Trichlorobenzene	34,2	288266	729459	1283242	2222498	3166380	158288	-108223	0,995
Hexachloro-1,3-butadiene	35,1	257850	740682	1170465	1948798	2692014	132148	-12379	0,996

Table 2. Five point calibration curve data.

Table 3 shows the summary data from 12 replicate runs of the calibration mix with analyte loading of 20 ppb@1L.

	R.T.	AVERAGE	Median	MIN	MAX	STD(n-1)	%RSD
Halocarbon 12	5,0	1154298	1126265	1078098	1309386	78121,5	7%
Chloromethane	5,6	121489	121894	110687	130155	6303,2	5%
Halocarbon 114	6,0	1755980	1750587	1609786	1899413	73239,8	4%
Vinyl Chloride	6,4	521388	521519,5	469652	566736	30020,1	6%
1,3-Butadiene	7,0	415879	412904	391197	439925	16398,0	4%
Bromomethane	7,9	403185	417611	326678	467091	43426,3	11%
Ethyl Chloride	8,6	87631	88084,5	77817	94606	4963,3	6%
Halocarbon 11	11,2	1783720	1781891	1707165	1852983	46548,9	3%
Acrylonitrile	11,9	330472	334410	298497	364673	19264,8	6%
1,1-Dichloroethylene	13,0	922068	924879,5	887006	940255	17122,4	2%
Methylene Chloride	13,2	601260	603345	563850	646004	22554,4	4%
3-Chloropropylene	13,6	309560	308206	291373	329149	12218,1	4%
Halocarbon 113	14,0	1748066	1732131	1694476	1851798	56562,3	3%
1,1 Dichloroethane	16,1	1158613	1147482	1114827	1229513	37060,5	3%
cis-1,2 Dichloroethane	17,9	827748	819539	800148	872497	22945,3	3%
Chloroform	18,5	1442897	1430803	1340918	1566810	61943,7	4%
1,2 Dichloroethane	20,0	785482	773317	752511	837671	30382,8	4%
1,1,1 Trichloroethane	20,6	1601450	1582115	1535761	1715836	61340,9	4%
Benzene	21,5	2453037	2442364	2312205	2588342	70614,3	3%
Carbon Tetrachloride	21,8	1829560	1809726	1746704	1980838	78972,9	4%
1,2-Dichloropropane	22,8	772768	774836,5	724920	804955	21196,9	3%
Trichloroethylene	23,2	1244495	1236981	1169404	1354731	52811,1	4%
cis-1,3 Dichloropropene	24,3	1189288	1197377	1050947	1266074	54272,2	5%
trans-1,3-Dichloropropene	25,0	894711	912775,5	765680	969569	57901,9	6%
1,1,2-Trichloroethane	25,3	1061067	1068008	912994	1128571	55459,6	5%
Toluene	25,6	3183621	3204893	2828758	3325931	128735,3	4%
1,2-Dibromoethane	26,5	1521604	1526443	1269738	1672651	97288,0	6%
Tetrachloroethylene	27,0	1919801	1958402	1580314	2067519	118254,4	6%
Chlorobenzene	27,7	2815144	2845633	2467791	2944808	131239,8	5%
Ethylbenzene	28,1	4121677	4217419	3365985	4349887	267981,4	7%
m,p-Xylene	28,3	6312395	6339619	5654139	6632478	248152,0	4%
Styrene	28,6	2390480	2401426	2116725	2504326	105590,6	4%
1,1,2,2-Tetrachlorethylene	28,8	1937346	1953214	1669794	2071979	126630,7	7%
o-xylene	28,8	3301755	3322176	2910746	3491193	144367,4	4%
4-Ethyltoluene	30,0	4148895	4134223	3846303	4539930	175205,0	4%
1,3,5-Trimethylbenzene	30,1	3972209	3973434	3865057	4133427	75031,1	2%
1,2,4-Trimethylbenzene	30,6	3989462	4025624	3720247	4174856	130298,2	3%
1,3-Dichlorobenzene	30,9	3295567	3296127	2997546	3617006	147249,3	4%
1,4-Dichlorobenzene	31,0	3305106	3316786	3124440	3640458	139984,7	4%
1,2-Dichlorobenzene	31,4	3077317	3092296	2811977	3400621	141154,5	5%
1,2,4-Trichlorobenzene	34,2	2843886	2895179	2571824	3067476	184664,3	6%
Hexachloro-1,3-butadiene	35,1	2495120	2500572	2328824	2811506	122110,5	5%

Table 3. Replicate analysis data.

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