The conversion of relative retention data into R_{x9} units

Retention data, which may be relative to any compound, may be converted into R_{x9} units[1] provided the relative retentions of at least four *n*-paraffins are included. Where retentions of *n*-paraffins are not included the direct conversion is not possible. However, it would not be difficult for the authors to determine R_{x9} values under similar column conditions.

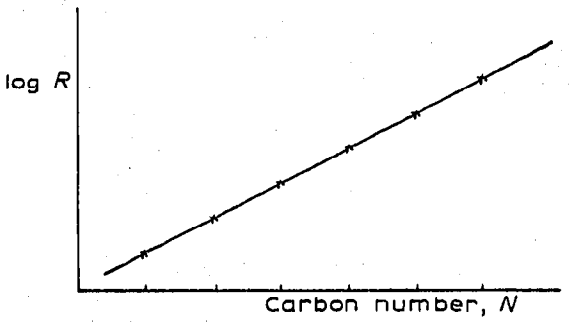

Fig. 1.

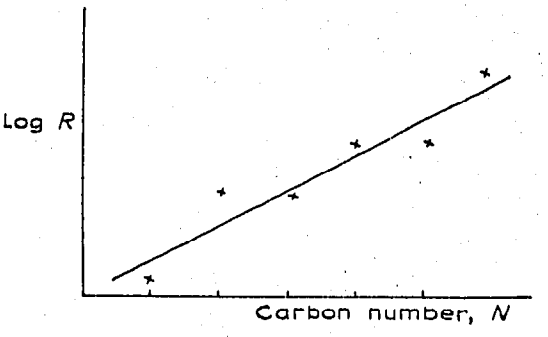

Fig. 2.

Published relative retention data fall into four types depending upon the nature of the "log plot" for the *n*-paraffins:

Case 1. The correct dead volume is taken (Fig. 1).

All the points fall on a straight line if the correct dead volume correction is applied. The value for *n*-nonane can be obtained by extra- or interpolation. This value is unity in R_{x9} units—the value for the original standard can then be calculated and all other data converted.

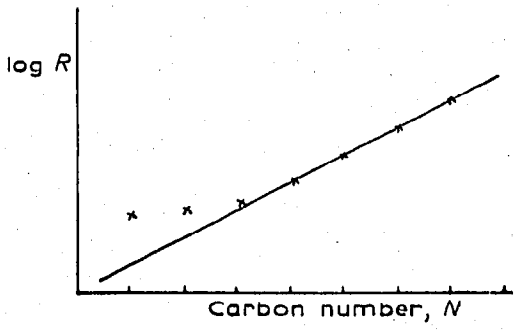

Fig. 3.

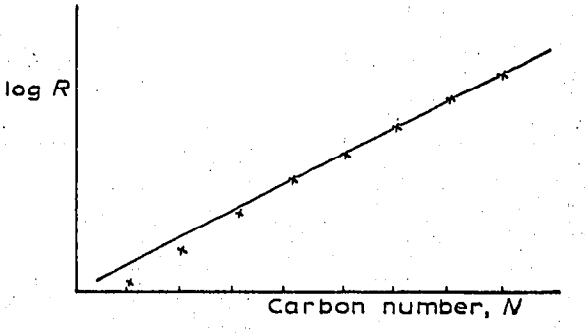

Fig. 4.

Case 2. Correct dead volume but random scatter (Fig. 2). Reflects poor technique or apparatus—data not worth conversion into R_{x9} units.

Case 3. Dead volume correction too small—as if measured from the point of injection (Fig. 3). The correct dead volume can be obtained by graphical linearization of the "log plot" or as outlined in the R_{x9} paper[1]. The R_{x9} values can then be calculated as in case 1.

Case 4. Dead volume correction too large—as if measured from the air peak (air has a significant retention[2]) (Fig. 4). The correct dead volume is obtained as for case 3.

TABLE I

THE CONVERSION OF RETENTION DATA RELATIVE TO *n*-PENTANE INTO R_{x_0} UNITS

20% by weight stationary phase on Chromosorb R, 60–80 mesh, length 4 m, temperature 50°.

Substance	*Di-isodecyl phthalate*	*Di-2-ethylhexyl sebacate*	*Silicone oil DC 200*	*Apiezon L*
Ethane	0.0013	0.0021	—	—
Propane	0.0029	0.0038	0.0054	0.0028
n-Butane	0.0078	0.0088	0.013	0.0077
n-Pentane	0.021	0.022	0.030	0.022
n-Hexane	0.056	0.061	0.073	0.052
n-Heptane	0.145	0.156	0.175	0.141
n-Octane	0.386	0.399	0.416	—
2-Methylpropane	0.0056	0.0066	0.0099	0.0051
2-Methylbutane	0.016	0.017	0.024	0.015
2-Methylpentane	0.043	0.044	0.057	0.038
Ethylene	0.0013	0.0021	0.0025	0.0012
Propylene	0.0034	0.0040	0.0054	0.0027
Isobutene	0.0083	0.0090	0.012	0.0065
But-1-ene	0.0083	0.0090	0.012	0.0065
trans-But-2-ene	0.011	0.011	0.014	0.0083
cis-But-2-ene	0.012	0.012	0.016	0.0092
Pent-1-ene	0.021	0.022	0.027	0.017
Hex-1-ene	0.059	0.058	0.066	0.046
trans-Pent-2-ene	0.026	0.026	0.032	0.021
cis-Pent-2-ene	0.027	0.028	0.034	0.022
trans-Hex-2-ene	0.065	0.066	0.075	0.052
cis-Hex-2-ene	0.072	0.072	0.083	0.057
Propadiene	0.0056	0.0062	0.0072	0.0038
But-1,3-diene	0.011	0.011	0.016	0.0072
2-Methylbut-1,3-diene	0.030	0.031	0.031	0.021
Acetylene	0.0018	0.0027	0.0027	0.0010
Propyne	0.0063	0.0056	0.0081	0.0036
But-1-yne	0.014	0.014	0.014	0.0072
Carbon dioxide	0.0013	0.0021	0.0022	0.0010
Neopentane	0.0090	0.0096	0.014	0.0076
Iso-octane	0.143	0.141	0.167	0.123

TABLE II

THE CONVERSION OF RETENTION DATA RELATIVE TO *n*-PENTANE INTO R_{x_0} UNITS

20% by weight stationary phase on Chromosorb R, 60–80 mesh, length 4 m, temperature 100°.

Substance	*Di-isodecyl phthalate*	*Di-2-ethylhexyl sebacate*	*Silicone oil DC 200*	*Apiezon L*
Ethane	—	0.0060	—	—
Propane	0.0078	0.011	0.019	—
n-Butane	0.019	0.024	0.037	0.021
n-Pentane	0.041	0.047	0.069	0.046
n-Hexane	0.093	0.103	0.136	0.100
n-Heptane	0.210	0.223	0.264	0.216
n-Octane	0.455	0.468	0.512	0.463

(continued on p. 543)

TABLE II (*continued*)

Substance	*Di-isodecyl phthalate*	*Di-2-ethylhexyl sebacate*	*Silicone oil DC 200*	*Apiezon L*
2-Methylpropane	0.015	0.019	0.029	0.015
2-Methylbutane	0.033	0.039	0.059	0.037
2-Methylpentane	0.073	0.082	0.107	0.078
Ethylene	0.0029	0.0048	0.0093	0.0031
Propylene	0.0087	0.011	0.019	0.0087
Isobutene	0.020	0.024	0.033	0.019
But-1-ene	0.020	0.024	0.033	0.019
trans-But-2-ene	0.025	0.029	0.037	0.023
cis-But-2-ene	0.027	0.031	0.043	0.025
Pent-1-ene	0.040	0.050	0.067	0.039
Hex-1-ene	0.093	0.104	0.123	0.087
trans-Pent-2-ene	0.044	0.053	0.069	0.047
cis-Pent-2-ene	0.047	0.059	0.075	0.049
trans-Hex-2-ene	0.103	0.115	0.139	0.100
cis-Hex-2-ene	0.109	0.122	0.147	0.106
Propadiene	0.015	0.019	0.026	0.013
But-1,3-diene	0.025	0.030	0.043	0.021
2-Methylbut-1,3-diene	0.054	0.062	0.064	0.049
Acetylene	0.0048	0.0072	0.011	0.0024
Propyne	0.015	0.020	0.024	0.014
But-1-yne	0.033	0.034	0.040	0.021
Benzene	0.250	0.258	0.205	0.115
Toluene	0.581	0.565	0.403	0.260
Ethylbenzene	1.13	1.09	0.798	0.504
p-Xylene	1.29	1.22	0.798	0.583
m-Xylene	1.29	1.22	0.798	0.583
o-Xylene	1.55	1.46	0.915	0.691
Isopropyl benzene	1.76	1.67	1.18	0.773
Cyclopentane	0.077	0.086	0.110	0.087
Methylcyclopentane	0.129	0.140	0.168	0.139
Cyclohexane	0.181	0.187	0.216	0.197
Methylcyclohexane	0.307	0.308	0.331	0.320
Methanol	0.070	0.056	0.059	0.035
Ethanol	0.093	0.077	0.059	0.058
n-Propanol	0.202	0.171	0.107	0.077
n-Butanol	0.466	0.392	0.219	0.202
Propan-2-ol	0.095	0.098	0.085	0.039
Butan-2-ol	0.214	0.228	0.160	0.110
tert.-Butanol	0.109	0.122	0.091	0.050
tert.-Pentanol	0.274	0.299	0.195	0.087
Acetaldehyde	0.039	0.034	0.040	0.011
Propionaldehyde	0.076	0.067	0.061	0.038
n-Butyraldehyde	0.159	0.144	0.117	0.090
n-Valeraldehyde	0.353	0.319	0.251	0.223

(continued on p. 544)

TABLE II (*continued*)

Substance	*Di-isodecyl phthalate*	*Di-2-ethylhexyl sebacate*	*Silicone oil DC 200*	*Apiezon L*
Acetone	0.085	0.071	0.075	0.038
Butan-2-one	0.175	0.151	0.133	0.099
Pentan-2-one	0.336	0.297	0.264	0.198
Heptan-2-one	1.48	—	0.877	0.497
Methyl acetate	0.087	0.079	0.104	0.047
Ethyl acetate	0.150	0.141	0.165	0.088
n-Propyl acetate	0.309	0.295	0.317	0.178
n-Butyl acetate	0.649	0.626	0.618	0.384
Diethyl ether	0.051	0.053	0.069	0.041
Di-isopropyl ether	0.101	0.108	0.133	0.077
Di-*n*-butyl ether	0.854	0.912	0.840	0.700
Carbon dioxide	—	0.0048	0.011	0.0024
Neopentane	0.021	0.026	0.043	0.020
Iso-octane	0.196	0.219	0.261	0.198
Water	0.124	0.086	0.144	0.129

As an illustration (see Tables I and II) we have converted the retention data of SCHOLLY AND BRENNER[3], which were measured from the air peak with *n*-pentane as standard. Corrections to the dead volume have been applied where necessary.

The Natural Rubber Producers' Research Association, Welwyn Garden City, Herts. (Great Britain)

M. B. EVANS
J. F. SMITH

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[2] J. F. SMITH, *Nature*, 193 (1962) 679.
[3] P. SCHOLLY AND N. BRENNER, *Proc. 2nd Intern. Symposium on Gas Chromatography*, Academic Press, New York, 1959, p. 263.

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Relative detector response in gas chromatography
IV. Ethers and acetals

The investigation of the relative detector response of a thermal conductivity detector to organic compounds of various types is continued with a study of the relative responses to aliphatic and cyclic ethers, and to aliphatic and cyclic acetals. MESSNER *et al.*[1], using helium as the carrier gas, found that the relative detector responses to aliphatic ethers increased with an increase in molecular weight and it has been shown previously[2–4] that, for other homologous series, there was such an increase in relative detector responses when nitrogen was used as the carrier gas.