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# Short Communication

# Structure–gas chromatographic retention time models of tetra-*n*-alkylsilanes and tetra-*n*-alkylgermanes using topological indexes

# A correction

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ABSTRACT

Previously reported [*J. Chromatogr.*, 630 (1993) 223] structure–gas chromatographic retention time models for 26 tetra-*n*-alkylsilanes, 26 tetra-*n*-alkylgermanes, and the mixed set of silanes and germanes have been corrected. Most of the previously reported equations are improved. The general conclusions of the previous paper remain unchanged.

## INTRODUCTION

In the author's previous paper [1] the topological indexes for compounds 15, 21, 41 and 47 in Table III were incorrectly computed. The analyses have been repeated using the correct topological indexes for these compounds.

## RESULTS

Equations 14, 15, 17 and 18 in the previous paper [1] are virtually unchanged. The other previously reported equations are improved and are given below. The numbers of the equations correspond to those in the previous paper [1]. The intercorrelation results are given after each multivariable equation. The results of the analysis using eqn. 20 are given in corrected Table III, which corresponds to Table III in the previous paper [1]:

$$\log T = -0.455(0.040) + 0.514(0.007)^1\chi \qquad (12)$$

$n = 26 \quad r = 0.998 \quad s = 0.045 \quad F = 5448$

$$\log T = -0.165(0.053) + 0.493(0.006)^1\chi - 0.193(0.031)^3\chi_c \qquad (13)$$

$n = 26 \quad r = 0.999 \quad s = 0.028 \quad F = 6959$

The intercorrelation between $^1\chi$ and $^3\chi_c$ is: $r = 0.627$

$$\log T = -0.029(0.052) + 0.490(0.006)^1\chi - 0.174(0.031)^3\chi_c \qquad (16)$$

$n = 26 \quad r = 0.999 \quad s = 0.027 \quad F = 7180$

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TABLE III

LOGARITHMS OF RETENTION TIMES OF TETRA-*n*-ALKYLSILANES AND TETRA-*n*-ALKYLGERMANES AND TOPOLOGICAL INDEXES

| No. | Compound[a] | $^1\chi$ | $^3\chi_c$ | $S$ | TTV | Log $T$[b] | Calc.[c] | Res.[d] |
|---|---|---|---|---|---|---|---|---|
| 1 | $Me_3BuSi$ | 3.5607 | 1.5607 | −0.6782 | 14.3584 | 1.29 | 1.31 | −0.02 |
| 2 | $MeEt_3Si$ | 3.6820 | 0.9286 | −0.6713 | 14.1734 | 1.43 | 1.48 | −0.05 |
| 3 | $Me_2Pr_2Si$ | 4.1213 | 1.2071 | −0.7033 | 17.2755 | 1.60 | 1.65 | −0.05 |
| 4 | $Me_2EtBuSi$ | 4.1213 | 1.2071 | −0.6982 | 17.2958 | 1.61 | 1.64 | −0.03 |
| 5 | $MeEt_2PrSi$ | 4.1820 | 0.9268 | −0.6973 | 17.2185 | 1.70 | 1.72 | −0.02 |
| 6 | $Et_4Si$ | 4.2426 | 0.7071 | −0.6914 | 17.1717 | 1.80 | 1.79 | 0.01 |
| 7 | $Me_2PrBuSi$ | 4.6213 | 1.2071 | −0.7243 | 20.3554 | 1.90 | 1.89 | 0.01 |
| 8 | $MeEtPr_2Si$ | 4.6820 | 0.9268 | −0.7234 | 20.2999 | 1.95 | 1.97 | −0.02 |
| 9 | $Et_3PrSi$ | 4.7426 | 0.7071 | −0.7174 | 20.2666 | 2.05 | 2.04 | 0.01 |
| 10 | $Me_2Bu_2Si$ | 5.1213 | 1.2071 | −0.7453 | 23.4573 | 2.15 | 2.13 | 0.02 |
| 11 | $MePr_3Si$ | 5.1820 | 0.9268 | −0.7494 | 23.4178 | 2.20 | 2.21 | −0.01 |
| 12 | $Et_2Pr_2Si$ | 5.2426 | 0.7071 | −0.7434 | 23.3979 | 2.29 | 2.28 | 0.01 |
| 13 | $Et_3BuSi$ | 5.2426 | 0.7071 | −0.7384 | 23.3913 | 2.32 | 2.28 | 0.04 |
| 14 | $MePr_2BuSi$ | 5.6820 | 0.9268 | −0.7704 | 26.5620 | 2.47 | 2.46 | 0.01 |
| 15 | $MeEtBu_2Si$ | 5.6820 | 0.9268 | −0.7653 | 26.5546 | 2.49 | 2.46 | 0.03 |
| 16 | $EtPr_3Si$ | 5.7426 | 0.7071 | −0.7695 | 26.5656 | 2.52 | 2.53 | −0.01 |
| 17 | $Pr_4Si$ | 6.2426 | 0.7071 | −0.7955 | 29.7698 | 2.74 | 2.77 | −0.03 |
| 18 | $EtPr_2BuSi$ | 6.2426 | 0.7071 | −0.7905 | 29.7462 | 2.77 | 2.77 | 0.00 |
| 19 | $Et_2Bu_2Si$ | 6.2426 | 0.7071 | −0.7854 | 29.7254 | 2.82 | 2.77 | 0.05 |
| 20 | $MeBu_3Si$ | 6.6820 | 0.9268 | −0.8123 | 32.9167 | 2.99 | 2.94 | 0.05 |
| 21 | $Pr_3BuSi$ | 6.7426 | 0.7071 | −0.8165 | 32.9782 | 2.99 | 3.02 | −0.03 |
| 22 | $EtPrBu_2Si$ | 6.7426 | 0.7071 | −0.8114 | 32.9489 | 3.03 | 3.01 | 0.02 |
| 23 | $Pr_2Bu_2Si$ | 7.2426 | 0.7071 | −0.8375 | 36.2088 | 3.24 | 3.26 | −0.02 |
| 24 | $EtBu_3Si$ | 7.2426 | 0.7071 | −0.8324 | 36.1737 | 3.30 | 3.26 | 0.04 |
| 25 | $PrBu_3Si$ | 7.7426 | 0.7071 | −0.8584 | 39.4616 | 3.49 | 3.50 | −0.01 |
| 26 | $Bu_4Si$ | 8.2426 | 0.7071 | −0.8794 | 42.7365 | 3.72 | 3.75 | −0.03 |
| 27 | $Me_3BuGe$ | 3.5607 | 1.5607 | −1.1086 | 13.4109 | 1.42 | 1.43 | −0.01 |
| 28 | $MeEt_3Ge$ | 3.6820 | 0.9268 | −1.1250 | 13.0229 | 1.57 | 1.60 | −0.03 |
| 29 | $Me_2Pr_2Ge$ | 4.1213 | 1.2071 | −1.1597 | 16.1384 | 1.77 | 1.77 | 0.00 |
| 30 | $Me_2EtBuGe$ | 4.1213 | 1.2071 | −1.1503 | 16.1933 | 1.77 | 1.77 | 0.00 |
| 31 | $MeEt_2PrGe$ | 4.1820 | 0.9286 | −1.1632 | 15.9902 | 1.84 | 1.85 | −0.01 |
| 32 | $Et_4Ge$ | 4.2426 | 0.7071 | −1.1667 | 15.8485 | 1.94 | 1.92 | 0.02 |
| 33 | $Me_2PrBuGe$ | 4.6213 | 1.2071 | −0.1885 | 19.1749 | 2.04 | 2.02 | 0.02 |
| 34 | $MeEtPr_2Ge$ | 4.6820 | 0.9268 | −1.2014 | 18.9886 | 2.09 | 2.10 | −0.01 |
| 35 | $Et_3PrGe$ | 4.7426 | 0.7071 | −1.2049 | 18.8569 | 2.18 | 2.17 | 0.01 |
| 36 | $Me_2Bu_2Ge$ | 5.1213 | 1.2071 | −1.2172 | 22.2309 | 2.31 | 2.26 | 0.05 |
| 37 | $MePr_3Ge$ | 5.1820 | 0.9268 | −1.2396 | 22.0178 | 2.35 | 2.35 | 0.00 |
| 38 | $Et_2Pr_2Ge$ | 5.2426 | 0.7071 | −1.2431 | 21.8963 | 2.42 | 2.42 | 0.00 |
| 39 | $Et_3BuGe$ | 5.2426 | 0.7071 | −1.2336 | 21.9310 | 2.45 | 2.42 | 0.03 |
| 40 | $MePr_2BuGe$ | 5.6820 | 0.9268 | −1.2683 | 25.1095 | 2.61 | 2.60 | 0.01 |
| 41 | $MeEtBu_2Ge$ | 5.6820 | 0.9268 | −1.2589 | 25.1429 | 2.64 | 2.59 | 0.05 |
| 42 | $EtPr_3Ge$ | 5.7426 | 0.7071 | −1.2813 | 24.9666 | 2.66 | 2.67 | −0.01 |
| 43 | $Pr_4Ge$ | 6.2426 | 0.7071 | −1.3194 | 28.0678 | 2.89 | 2.92 | −0.03 |
| 44 | $EtPr_2BuGe$ | 6.2426 | 0.7071 | −1.3100 | 28.0891 | 2.91 | 2.91 | 0.00 |
| 45 | $Et_2Bu_2Ge$ | 6.2426 | 0.7071 | −1.3006 | 28.1125 | 2.95 | 2.91 | 0.04 |
| 46 | $MeBu_3Ge$ | 6.6820 | 0.9268 | −1.3258 | 31.3514 | 3.14 | 3.09 | 0.05 |
| 47 | $Pr_3BuGe$ | 6.7426 | 0.7071 | −1.3482 | 31.2146 | 3.13 | 3.16 | −0.03 |
| 48 | $EtPrBu_2Ge$ | 6.7426 | 0.7071 | −1.3388 | 31.2313 | 3.16 | 3.16 | 0.00 |
| 49 | $Pr_2Bu_2Ge$ | 7.2426 | 0.7071 | −1.3769 | 34.3810 | 3.38 | 3.41 | −0.03 |
| 50 | $EtBu_3Ge$ | 7.2426 | 0.7071 | −1.3675 | 34.3930 | 3.40 | 3.41 | −0.01 |
| 51 | $PrBu_3Ge$ | 7.7426 | 0.7071 | −1.4057 | 37.5670 | 3.61 | 3.65 | −0.04 |
| 52 | $Bu_4Ge$ | 8.2426 | 0.7071 | −1.4344 | 40.7725 | 3.85 | 3.90 | −0.05 |

[a] Me = Methyl; Et = ethyl; Pr = *n*-propyl; Bu = *n*-butyl.
[b] Logarithm of retention time taken from ref. 24.
[c] Calculated from eqn. 20.
[d] Residual = Log $T$ − calc.

The intercorrelation between $^{1}\chi$ and $^{3}\chi_{c}$ is: $r = 0.627$

$$\log T = -0.468(0.022) + 0.485(0.004)^{1}\chi + 0.023(0.001)^{3}\chi^{v} \quad (19)$$

$n = 52$ $r = 0.999$ $s = 0.033$ $F = 9810$

The intercorrelation between $^{1}\chi$ and $^{3}\chi^{v}$ is: $r = -0.420$

$$\log T = -0.290(0.040) + 0.476(0.004)^{1}\chi - 0.183(0.023)^{3}\chi_{c} - 0.277(0.016)S \quad (20)$$

$n = 52$ $r = 0.999$ $s = 0.029$ $F = 8850$

The intercorrelation results are: $r = 0.218$ for $S$ and $^{1}\chi$, $r = -0.001$ for $S$ and $^{3}\chi_{c}$, and $r = 0.612$ for $^{1}\chi$ and $^{3}\chi_{c}$.

$$\log T = -1.265(0.030) + 0.372(0.003)^{0}\chi^{r} + 0.040(0.002)^{4}\chi^{v}_{pc} \quad (21)$$

$n = 52$ $r = 0.999$ $s = 0.034$ $F = 9478$

The intercorrelation between $^{0}\chi^{r}$ and $^{4}\chi^{v}_{pc}$ is: $r = 0.010$.

## REFERENCE

1 E.J. Kupchik, *J. Chromatogr.*, 630 (1993) 223.