

## Data material for

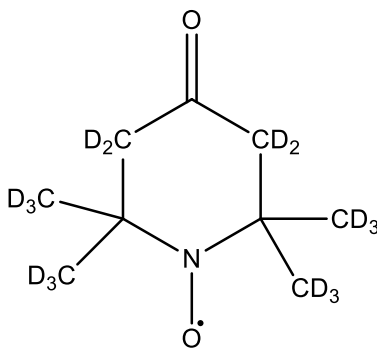
### “Comparing Radical Diffusion Crossover Phenomena in Alcohols and Alkanes”

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In this work, we applied electron spin resonance (ESR) to study translational diffusion of nitroxide radical 4-oxo-2,2,6,6-tetramethylpiperidine-d<sub>16</sub>-1-oxyl or perdeuterated TEMPONE (Figure 1), which was dissolved in two series of liquids. We determined tracer diffusion coefficients or tracer diffusivities  $D_T$  of perdeuterated TEMPONE at various temperatures in the normal alkane series from octane to tridecane (Tables 1 and 2) and the normal alcohol series from methanol to 1-octanol (Tables 3 and 4).

**Figure 1.** Chemical structure of perdeuterated TEMPONE radical



**Table 1.** Tracer diffusivities  $D_T$  and errors  $dD_T$  of perdeuterated TEMPONE radical in normal alkane series from octane to decane.

| $T$<br>°C | octane                      |                              | nonane                      |                              | decane                      |                              |
|-----------|-----------------------------|------------------------------|-----------------------------|------------------------------|-----------------------------|------------------------------|
|           | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns |
| 50        |                             |                              |                             |                              | 145.44                      | 0.24                         |
| 45        |                             |                              |                             |                              | 136.97                      | 2.43                         |
| 40        |                             |                              | 148.52                      | 2.51                         | 127.88                      | 1.43                         |
| 35        |                             |                              | 138.50                      | 1.29                         | 119.42                      | 2.47                         |
| 30        |                             |                              | 130.98                      | 0.38                         | 110.71                      | 1.97                         |
| 25        | 148.12                      | 1.78                         | 123.50                      | 0.12                         | 104.27                      | 2.72                         |
| 20        | 140.52                      | 1.61                         | 115.43                      | 1.73                         | 97.98                       | 1.54                         |
| 15        | 129.50                      | 1.96                         | 108.08                      | 0.53                         | 90.29                       | 1.45                         |
| 10        | 121.70                      | 1.53                         | 99.25                       | 0.35                         | 82.88                       | 0.82                         |
| 5         | 112.95                      | 2.83                         | 92.18                       | 0.25                         | 76.96                       | 1.01                         |
| 0         | 106.23                      | 3.62                         | 84.40                       | 0.01                         | 69.16                       | 2.26                         |
| -5        | 98.13                       | 1.84                         | 79.56                       | 1.09                         | 64.87                       | 0.34                         |
| -10       | 90.60                       | 2.55                         | 72.87                       | 1.22                         | 59.95                       | 0.56                         |
| -15       | 83.31                       | 1.38                         | 66.40                       | 1.95                         | 54.07                       | 1.56                         |
| -20       | 77.54                       | 2.80                         | 60.24                       | 0.93                         | 49.00                       | 0.78                         |
| -25       | 72.83                       | 1.31                         | 55.72                       | 1.39                         | 44.83                       | 1.55                         |
| -30       | 68.20                       | 2.99                         | 51.38                       | 1.46                         | 41.71                       | 0.95                         |
| -35       | 62.29                       | 2.11                         | 47.47                       | 2.89                         |                             |                              |
| -40       | 56.15                       | 0.21                         | 42.91                       | 1.91                         |                             |                              |
| -45       | 54.27                       | 2.05                         | 38.18                       | 1.91                         |                             |                              |
| -50       | 49.65                       | 0.11                         | 33.91                       | 1.29                         |                             |                              |
| -55       | 44.75                       | 1.30                         |                             |                              |                             |                              |

**Table 2.** Tracer diffusivities  $D_T$  and errors  $dD_T$  of perdeuterated TEMPONE radical in normal alkane series from undecane to tridecane.

| $T$<br>°C | undecane                    |                              | dodecane                    |                              | tridecane                   |                              |
|-----------|-----------------------------|------------------------------|-----------------------------|------------------------------|-----------------------------|------------------------------|
|           | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns |
| 80        |                             |                              |                             |                              | 142.74                      | 0.23                         |
| 75        |                             |                              |                             |                              | 133.61                      | 0.80                         |
| 70        |                             |                              | 143.35                      | 3.62                         | 127.06                      | 2.24                         |
| 65        |                             |                              | 134.99                      | 3.31                         | 119.11                      | 0.46                         |
| 60        | 147.84                      | 0.07                         | 126.33                      | 2.13                         | 111.82                      | 0.94                         |
| 55        | 139.41                      | 2.23                         | 119.52                      | 2.93                         | 103.79                      | 1.30                         |
| 50        | 129.40                      | 1.23                         | 112.66                      | 3.03                         | 98.84                       | 0.15                         |
| 45        | 122.57                      | 0.64                         | 104.70                      | 1.63                         | 91.44                       | 1.42                         |
| 40        | 113.96                      | 1.15                         | 98.54                       | 1.87                         | 84.29                       | 1.44                         |
| 35        | 106.20                      | 0.33                         | 90.90                       | 0.99                         | 79.56                       | 0.63                         |
| 30        | 101.00                      | 0.77                         | 85.12                       | 0.42                         | 72.32                       | 0.32                         |
| 25        | 92.63                       | 1.08                         | 78.03                       | 1.60                         | 67.14                       | 0.95                         |
| 20        | 85.88                       | 0.03                         | 71.56                       | 1.09                         | 62.22                       | 0.59                         |
| 15        | 79.37                       | 0.60                         | 66.12                       | 0.11                         | 57.50                       | 1.97                         |
| 10        | 72.63                       | 2.19                         | 60.55                       | 0.89                         | 53.15                       | 0.59                         |
| 5         | 68.60                       | 0.37                         | 55.59                       | 0.63                         | 47.75                       | 1.91                         |
| 0         | 61.50                       | 1.58                         | 50.32                       | 1.62                         | 43.82                       | 1.44                         |
| -5        | 56.92                       | 0.46                         | 45.42                       | 1.68                         | 39.34                       | 1.12                         |
| -10       | 50.65                       | 1.63                         | 41.16                       | 0.99                         |                             |                              |
| -15       | 46.67                       | 1.46                         |                             |                              |                             |                              |
| -20       | 41.91                       | 1.49                         |                             |                              |                             |                              |
| -25       | 38.87                       | 1.73                         |                             |                              |                             |                              |

**Table 3.** Tracer diffusivities  $D_T$  and errors  $dD_T$  of perdeuterated TEMPONE radical in normal alcohol series from methanol to 1-butanol.

| $T$<br>°C | methanol                    |                              | ethanol                     |                              | 1-propanol                  |                              | 1-butanol                   |                              |
|-----------|-----------------------------|------------------------------|-----------------------------|------------------------------|-----------------------------|------------------------------|-----------------------------|------------------------------|
|           | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns |
| 100       |                             |                              |                             |                              |                             |                              | 149.40                      | 2.17                         |
| 95        |                             |                              |                             |                              |                             |                              | 132.41                      | 0.87                         |
| 90        |                             |                              |                             |                              |                             |                              | 120.30                      | 3.22                         |
| 85        |                             |                              |                             |                              |                             |                              | 112.95                      | 0.33                         |
| 80        |                             |                              |                             |                              | 126.77                      | 1.76                         | 105.92                      | 0.02                         |
| 75        |                             |                              |                             |                              | 115.97                      | 2.39                         | 97.24                       | 0.04                         |
| 70        |                             |                              |                             |                              | 108.39                      | 1.77                         | 91.52                       | 0.84                         |
| 65        |                             |                              |                             |                              | 99.51                       | 1.61                         | 83.27                       | 1.76                         |
| 60        |                             |                              | 115.03                      | 8.92                         | 91.60                       | 1.69                         | 77.32                       | 1.12                         |
| 55        |                             |                              | 108.63                      | 6.04                         | 84.80                       | 1.54                         | 70.15                       | 0.42                         |
| 50        | 136.13                      | 10.04                        | 104.31                      | 10.60                        | 77.91                       | 1.91                         | 64.57                       | 0.81                         |
| 45        | 127.48                      | 8.66                         | 90.87                       | 6.07                         | 71.63                       | 1.22                         | 59.78                       | 1.17                         |
| 40        | 117.26                      | 5.83                         | 86.91                       | 5.51                         | 66.45                       | 1.04                         | 54.67                       | 2.03                         |
| 35        | 108.93                      | 5.77                         | 79.32                       | 7.58                         | 61.22                       | 1.08                         | 51.41                       | 0.62                         |
| 30        | 101.80                      | 5.00                         | 74.41                       | 3.84                         | 55.56                       | 0.54                         | 46.65                       | 0.54                         |
| 25        | 98.34                       | 3.78                         | 67.95                       | 3.97                         | 50.29                       | 1.02                         | 42.05                       | 1.24                         |
| 20        | 89.58                       | 6.54                         | 64.24                       | 3.36                         | 47.47                       | 1.36                         | 39.16                       | 1.90                         |
| 15        | 82.87                       | 6.67                         | 57.52                       | 1.53                         | 42.85                       | 1.65                         | 35.37                       | 1.17                         |
| 10        | 75.06                       | 3.62                         | 52.02                       | 0.56                         | 37.62                       | 1.16                         | 32.89                       | 1.47                         |
| 5         | 70.86                       | 3.57                         | 49.04                       | 0.31                         | 35.14                       | 1.40                         | 29.80                       | 0.72                         |
| 0         | 65.68                       | 2.41                         | 44.56                       | 0.36                         | 32.36                       | 0.51                         | 27.21                       | 0.27                         |
| -5        | 63.20                       | 2.07                         | 40.97                       | 0.81                         | 28.90                       | 1.21                         | 23.55                       | 0.15                         |
| -10       | 56.87                       | 0.44                         | 38.08                       | 1.07                         | 26.73                       | 0.92                         | 21.68                       | 1.03                         |
| -15       | 53.94                       | 1.09                         | 35.25                       | 0.97                         | 23.00                       | 0.40                         | 18.30                       | 1.50                         |
| -20       | 50.16                       | 0.84                         | 32.37                       | 1.05                         | 20.50                       | 1.65                         | 15.95                       | 2.55                         |
| -25       | 45.55                       | 2.49                         | 28.40                       | 0.09                         | 17.68                       | 1.43                         | 13.60                       | 3.25                         |
| -30       | 43.31                       | 0.23                         | 26.21                       | 0.09                         | 16.00                       | 1.35                         | 10.30                       | 1.80                         |
| -35       | 40.99                       | 1.11                         | 23.88                       | 0.67                         | 12.63                       | 1.23                         | 8.15                        | 2.00                         |
| -40       | 37.76                       | 2.53                         | 20.80                       | 0.70                         | 10.43                       | 1.48                         |                             |                              |
| -45       | 35.95                       | 2.52                         | 18.25                       | 1.15                         | 7.95                        | 1.35                         |                             |                              |
| -50       | 33.94                       | 2.37                         | 17.30                       | 1.45                         |                             |                              |                             |                              |
| -55       | 30.09                       | 1.81                         | 14.18                       | 0.78                         |                             |                              |                             |                              |
| -60       | 26.74                       | 0.97                         | 11.73                       | 1.67                         |                             |                              |                             |                              |
| -65       | 24.82                       | 1.32                         | 9.35                        | 1.85                         |                             |                              |                             |                              |
| -70       | 21.53                       | 2.51                         | 7.55                        | 1.90                         |                             |                              |                             |                              |
| -75       | 22.23                       | 0.73                         |                             |                              |                             |                              |                             |                              |
| -80       | 16.93                       | 1.88                         |                             |                              |                             |                              |                             |                              |
| -85       | 11.98                       | 0.88                         |                             |                              |                             |                              |                             |                              |

**Table 3.** Tracer diffusivities  $D_T$  and errors  $dD_T$  of perdeuterated TEMPONE radical in normal alcohol series from 1-pentanol to 1-octanol.

| $T$<br>°C | 1-pentanol                  |                              | 1-hexanol                   |                              | 1-heptanol                  |                              | 1-octanol                   |                              |
|-----------|-----------------------------|------------------------------|-----------------------------|------------------------------|-----------------------------|------------------------------|-----------------------------|------------------------------|
|           | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns | $D_T$<br>Å <sup>2</sup> /ns | $dD_T$<br>Å <sup>2</sup> /ns |
| 100       | 130.58                      | 2.11                         | 122.07                      | 0.24                         | 109.86                      | 1.28                         | 105.53                      | 1.27                         |
| 95        | 120.68                      | 3.53                         | 113.64                      | 1.68                         | 100.89                      | 2.54                         | 97.55                       | 4.02                         |
| 90        | 114.20                      | 2.57                         | 101.72                      | 1.04                         | 92.90                       | 2.28                         | 88.62                       | 2.32                         |
| 85        | 104.07                      | 2.35                         | 98.44                       | 2.57                         | 87.26                       | 2.21                         | 82.65                       | 2.18                         |
| 80        | 97.70                       | 1.20                         | 87.27                       | 0.11                         | 80.41                       | 3.01                         | 75.50                       | 2.01                         |
| 75        | 89.68                       | 2.05                         | 81.64                       | 0.01                         | 73.77                       | 2.18                         | 69.80                       | 1.75                         |
| 70        | 84.44                       | 1.10                         | 73.88                       | 2.27                         | 67.78                       | 2.32                         | 63.28                       | 2.02                         |
| 65        | 76.45                       | 2.20                         | 68.17                       | 1.25                         | 61.79                       | 1.22                         | 57.68                       | 1.96                         |
| 60        | 69.98                       | 2.98                         | 62.72                       | 0.84                         | 57.26                       | 1.87                         | 53.31                       | 1.66                         |
| 55        | 65.46                       | 1.75                         | 56.62                       | 0.75                         | 52.63                       | 2.25                         | 48.41                       | 1.43                         |
| 50        | 58.27                       | 1.69                         | 53.11                       | 1.59                         | 48.01                       | 1.42                         | 43.90                       | 1.59                         |
| 45        | 53.95                       | 2.61                         | 48.49                       | 2.35                         | 43.54                       | 2.19                         | 40.60                       | 1.26                         |
| 40        | 50.14                       | 2.47                         | 43.82                       | 1.40                         | 38.91                       | 1.05                         | 36.74                       | 0.67                         |
| 35        | 46.17                       | 2.73                         | 40.82                       | 1.02                         | 35.05                       | 0.95                         | 32.89                       | 0.04                         |
| 30        | 41.11                       | 2.47                         | 37.00                       | 0.56                         | 32.27                       | 0.25                         | 29.70                       | 0.20                         |
| 25        | 37.99                       | 2.15                         | 33.71                       | 0.17                         | 28.90                       | 0.25                         | 26.96                       | 0.52                         |
| 20        | 33.81                       | 1.96                         | 30.66                       | 0.34                         | 24.63                       | 1.68                         | 22.53                       | 1.22                         |
| 15        | 31.27                       | 1.04                         | 27.28                       | 0.99                         | 20.63                       | 0.32                         | 19.70                       | 1.95                         |
| 10        | 28.21                       | 0.41                         | 23.08                       | 1.13                         | 16.48                       | 0.42                         | 15.73                       | 2.23                         |
| 5         | 23.98                       | 0.27                         | 20.35                       | 2.00                         | 13.13                       | 0.33                         | 12.68                       | 1.93                         |
| 0         | 21.03                       | 0.07                         | 16.95                       | 2.75                         | 10.75                       | 0.50                         | 9.30                        | 1.40                         |
| -5        | 18.23                       | 0.78                         | 14.13                       | 2.97                         | 8.10                        | 0.80                         | 7.48                        | 0.52                         |
| -10       | 14.75                       | 1.60                         | 10.90                       | 2.60                         | 5.80                        | 0.85                         | 5.23                        | 0.38                         |
| -15       | 12.35                       | 1.05                         | 8.43                        | 2.57                         |                             |                              |                             |                              |
| -20       | 8.98                        | 0.83                         |                             |                              |                             |                              |                             |                              |
| -25       | 7.15                        | 0.50                         |                             |                              |                             |                              |                             |                              |