

## Supplementary Material

### Isoparametricity and related phenomena in reactions of *trans*-2,3-diaryloxiranes with arenesulfonic acids

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## Kinetic Data

**Table S1.** Rate constants  $k_{XYT} \times 10^5$ ,  $M^{-2} s^{-1}$ , values of  $q_Y^{XT}$  ( $r \geq 0.992$ ) in equation  $\log k_{XYT} = \log k_{XOT} + q_Y^{XT} \sigma_Y$  and  $q_X^{YT}$  ( $r \geq 0.992$ ) in equation  $\log k_{XYT} = \log k_{OYT} + q_X^{YT} \tau_X$  for reactions of *trans*-2,3-diaryloxiranes **1a–1d** with arenesulfonic acids **2a–2e** in the mixture dioxane–1,2-dichloroethane (7 : 3, v : v) at different temperatures  $T^{17}$

| Acid ( $\sigma_Y$ ) | Oxirane ( $\tau_X$ ) |                  |                  |                   | $-q_X^{YT}$       |
|---------------------|----------------------|------------------|------------------|-------------------|-------------------|
|                     | <b>1a</b> (0)        | <b>1b</b> (2.02) | <b>1c</b> (3.47) | <b>1d</b> (4.38)  |                   |
| $T = 265 \text{ K}$ |                      |                  |                  |                   |                   |
| <b>2a</b> (-0.27)   | $2120 \pm 80$        | $31.06 \pm 0.06$ | $1.51 \pm 0.07$  | $0.225 \pm 0.001$ | $0.908 \pm 0.001$ |
| <b>2b</b> (-0.17)   | $3000 \pm 100$       | $39.3 \pm 0.2$   | $1.66 \pm 0.01$  | $0.227 \pm 0.002$ | $0.941 \pm 0.002$ |
| <b>2c</b> (0)       | $5700 \pm 100$       | $55 \pm 1$       | $1.95 \pm 0.05$  | $0.238 \pm 0.002$ | $0.996 \pm 0.003$ |
| <b>2d</b> (0.23)    | $12900 \pm 300$      | $100 \pm 2$      | $2.37 \pm 0.06$  | $0.253 \pm 0.006$ | $1.08 \pm 0.01$   |
| <b>2e</b> (0.71)    | -                    | -                | $4.67 \pm 0.03$  | -                 |                   |
| $q_Y^{XT}$          | $1.57 \pm 0.02$      | $1.00 \pm 0.04$  | $0.50 \pm 0.03$  | $0.10 \pm 0.05$   |                   |
| $T = 281 \text{ K}$ |                      |                  |                  |                   |                   |
| <b>2a</b>           | $4900 \pm 300$       | -                | $4.6 \pm 0.2$    | $1.51 \pm 0.01$   | $0.82 \pm 0.06$   |
| <b>2b</b>           | $7500 \pm 200$       | -                | $6.36 \pm 0.09$  | $1.80 \pm 0.02$   | $0.84 \pm 0.05$   |
| <b>2c</b>           | $16600 \pm 200$      | -                | $9.8 \pm 0.2$    | $2.21 \pm 0.03$   | $0.90 \pm 0.04$   |
| <b>2d</b>           | $47900 \pm 500$      | -                | $18 \pm 1$       | $2.75 \pm 0.05$   | $0.97 \pm 0.01$   |
| <b>2e</b>           | -                    | -                | $54.2 \pm 0.4$   | -                 |                   |
| $q_Y^{XT}$          | $1.98 \pm 0.01$      |                  | $1.08 \pm 0.03$  | $0.50 \pm 0.04$   |                   |
| $T = 298 \text{ K}$ |                      |                  |                  |                   |                   |
| <b>2a</b>           | $8320 \pm 400$       | -                | $24.3 \pm 0.9$   | $9.86 \pm 0.04$   | $0.68 \pm 0.05$   |
| <b>2b</b>           | $13010 \pm 100$      | -                | $32.0 \pm 0.4$   | $12.1 \pm 0.2$    | $0.71 \pm 0.05$   |
| <b>2c</b>           | $32700 \pm 500$      | -                | $52.2 \pm 0.5$   | $20.2 \pm 0.1$    | $0.75 \pm 0.06$   |
| <b>2d</b>           | $142000 \pm 100$     | -                | $117 \pm 3$      | $29.8 \pm 0.1$    | $0.85 \pm 0.04$   |
| <b>2e</b>           | -                    | -                | $690 \pm 20$     | -                 |                   |
| $q_Y^{XT}$          | $2.5 \pm 0.1$        |                  | $1.49 \pm 0.05$  | $1.01 \pm 0.09$   |                   |

## Activation Data

**Table S2.** Values of coefficients of Eyring equation<sup>a</sup> ( $r \geq 0.989$ ) and activation parameters  $\Delta H_{XY}^\ddagger$  (kJ mol<sup>-1</sup>),  $\Delta S_{XY}^\ddagger$  (J mol<sup>-1</sup> K<sup>-1</sup>) and  $\Delta G_{XYT}^\ddagger$  (kJ mol<sup>-1</sup>) for reactions of *trans*-2,3-diaryloxiranes with arenesulfonic acids in the mixture of dioxane with 1,2-dichloroethane (7 : 3 v/v) at 265, 281, and 298 K<sup>17</sup>

| Acid              | $A_{T=\infty}^{XY}$ | $-B_T^{XY}$ | $\Delta H_{XY}^\ddagger$ | $\Delta S_{XY}^\ddagger$ | $\Delta G_{XYT=265}^\ddagger$ | $\Delta G_{XYT=281}^\ddagger$ | $\Delta G_{XYT=298}^\ddagger$ |
|-------------------|---------------------|-------------|--------------------------|--------------------------|-------------------------------|-------------------------------|-------------------------------|
| Oxirane <b>1a</b> |                     |             |                          |                          |                               |                               |                               |
| <b>2a</b>         | 1.0 ± 0.6           | 1.3 ± 0.2   | 25                       | -178                     | 72.2                          | 75.0                          | 78.0                          |
| <b>2b</b>         | 1.5 ± 0.8           | 1.4 ± 0.2   | 27                       | -169                     | 71.8                          | 74.5                          | 77.4                          |
| <b>2c</b>         | 2.9 ± 0.8           | 1.7 ± 0.2   | 32                       | -142                     | 69.6                          | 71.9                          | 74.3                          |
| <b>2d</b>         | 5.8 ± 0.3           | 2.41 ± 0.09 | 46                       | -86                      | 68.8                          | 70.2                          | 71.6                          |
| Oxirane <b>1c</b> |                     |             |                          |                          |                               |                               |                               |
| <b>2a</b>         | 3 ± 1               | 2.8 ± 0.4   | 53                       | -140                     | 90.1                          | 92.3                          | 94.7                          |
| <b>2b</b>         | 4.1 ± 0.7           | 3.0 ± 0.2   | 57                       | -121                     | 89.1                          | 91.0                          | 93.1                          |
| <b>2c</b>         | 5.87 ± 0.07         | 3.46 ± 0.02 | 66                       | -86                      | 88.8                          | 90.2                          | 91.6                          |
| <b>2d</b>         | 8.1 ± 0.1           | 4.02 ± 0.04 | 77                       | -42                      | 88.1                          | 88.8                          | 89.5                          |
| <b>2e</b>         | 12.6 ± 0.4          | 5.1 ± 0.1   | 98                       | 44                       | 86.3                          | 85.6                          | 84.9                          |
| Oxirane <b>1d</b> |                     |             |                          |                          |                               |                               |                               |
| <b>2a</b>         | 6.5 ± 0.1           | 3.88 ± 0.04 | 74                       | -73                      | 93.3                          | 94.5                          | 95.7                          |
| <b>2b</b>         | 7.4 ± 0.2           | 4.10 ± 0.05 | 78                       | -56                      | 92.8                          | 94.0                          | 94.7                          |
| <b>2c</b>         | 9.2 ± 0.1           | 4.58 ± 0.04 | 88                       | -19                      | 93.6                          | 93.9                          | 94.2                          |
| <b>2d</b>         | 10.5 ± 0.2          | 4.92 ± 0.07 | 94                       | 3.4                      | 93.1                          | 93.0                          | 93.0                          |

<sup>a</sup>  $\log (k_{XYT}/T) = A_{T=\infty}^{XY} + B_T^{XY} \cdot 10^3/T$ , here  $A_{T=\infty}^{XY} = \lg(k_B/h) + \Delta S_{XY}^\ddagger/2.3R$ ,  $B_T^{XY} = -\Delta H_{XY}^\ddagger/2.3R$  ( $k_B$  is Boltzmann constant,  $h$  is Plank constant,  $R$  is a gas constant).