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A-2134-1**Table S1.**  $^1\text{H}$  NMR Chemical Shifts of H1 in Titrations of Mixtures of Stereoisomeric 4-*t*-Butylcyclohexylamines (1) with DCl in DMSO- $d_6$  at 25° C.

|      | 0.20 M     |            | 0.10 M     |            | 0.05 M     |            |
|------|------------|------------|------------|------------|------------|------------|
| titr | $\delta_c$ | $\delta_t$ | $\delta_c$ | $\delta_t$ | $\delta_c$ | $\delta_t$ |
| 0    | 3.040      | 2.402      | 3.039      | 2.401      | 3.037      | 2.400      |
| 1    | 3.063      | 2.456      | 3.067      | 2.467      | 3.067      | 2.467      |
| 2    | 3.086      | 2.508      | 3.098      | 2.532      | 3.117      | 2.572      |
| 3    | 3.118      | 2.571      | 3.132      | 2.596      | 3.165      | 2.652      |
| 4    | 3.147      | 2.620      | 3.169      | 2.657      | 3.212      | 2.722      |
| 5    | 3.176      | 2.668      | 3.213      | 2.720      | 3.275      | 2.800      |
| 6    | 3.212      | 2.720      | 3.254      | 2.775      | 3.335      | 2.865      |
| 7    | 3.252      | 2.773      | 3.312      | 2.840      | 3.373      | 2.902      |
| 8    | 3.292      | 2.821      | 3.363      | 2.890      |            |            |
| 9    | 3.339      | 2.868      | 3.373      | 2.901      |            |            |
| 10   | 3.372      | 2.901      |            |            |            |            |

**Table S2.**  $^1\text{H}$  NMR Chemical Shifts of H1 in a Titration of *cis* and *trans* stereoisomers of 4-*t*-Butylcyclohexanecarboxylic Acid (2) with NaOD in 3:1 CD<sub>3</sub>OD/D<sub>2</sub>O at 25° C.

| titr | $\delta_c$ | $\delta_t$ | titr | $\delta_c$ | $\delta_t$ | titr | $\delta_c$ | $\delta_t$ |
|------|------------|------------|------|------------|------------|------|------------|------------|
| 0    | 2.186      | 2.629      | 7    | 2.117      | 2.581      | 14   | 2.056      | 2.496      |
| 1    | 2.178      | 2.624      | 8    | 2.109      | 2.573      | 15   | 2.052      | 2.485      |
| 2    | 2.162      | 2.615      | 9    | 2.102      | 2.566      | 16   | 2.042      | 2.460      |
| 3    | 2.153      | 2.609      | 10   | 2.094      | 2.557      | 17   | 2.036      | 2.444      |
| 4    | 2.140      | 2.601      | 11   | 2.090      | 2.550      | 18   | 2.028      | 2.417      |
| 5    | 2.133      | 2.595      | 12   | 2.083      | 2.541      | 19   | 2.025      | 2.408      |
| 6    | 2.127      | 2.590      | 13   | 2.065      | 2.513      | 20   | 2.022      | 2.396      |

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**Table S3.**  $^{13}\text{C}$  NMR Chemical Shifts in a Titration of a Mixture of *cis* and *trans* stereoisomers of 4-*t*-Butylcyclohexanecarboxylic Acid (**2**) with NaOD in 3:1  $\text{CD}_3\text{OD}/\text{D}_2\text{O}$  at 25° C.

| titr | $\delta_{\text{c-CO}}$ | $\delta_{\text{t-CO}}$ | $\delta_{\text{c-C1}}$ | $\delta_{\text{t-C1}}$ | $\delta_{\text{c-C2}}$ | $\delta_{\text{t-C2}}$ | $\delta_{\text{c-C4}}$ | $\delta_{\text{t-C4}}$ |
|------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| 0    | 178.376                | 179.590                | 38.486                 | 43.145                 | 27.317                 | 29.177                 | 47.614                 | 47.215                 |
| 1    | 179.038                | 181.301                | 38.844                 | 44.408                 | 27.496                 | 29.511                 | 47.694                 | 47.281                 |
| 2    | 179.951                | 182.771                | 39.338                 | 45.495                 | 27.751                 | 29.805                 | 47.816                 | 47.351                 |
| 3    | 181.226                | 184.000                | 40.029                 | 46.397                 | 28.108                 | 30.057                 | 47.987                 | 47.404                 |
| 4    | 182.446                | 184.735                | 40.691                 | 46.949                 | 28.442                 | 30.202                 | 48.139                 | 47.435                 |
| 5    | 183.126                | 185.044                | 41.055                 | 47.174                 | 28.618                 | 30.257                 | 48.230                 | 47.447                 |

**Table S4.**  $^1\text{H}$  NMR Chemical Shifts of H1 in a Titration of a Mixture of *cis* and *trans* stereoisomers of 4-*t*-Butylcyclohexanecarboxylic Acid (**2**) with NaOD in 3:1  $\text{CD}_3\text{OD}/\text{D}_2\text{O}$ .

| titr | 15° C               |                     | 22° C               |                     | 33° C               |                     | 41° C               |                     | 56° C               |                     |
|------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
|      | $\delta_{\text{c}}$ | $\delta_{\text{t}}$ | $\delta_{\text{c}}$ | $\delta_{\text{t}}$ | $\delta_{\text{c}}$ | $\delta_{\text{t}}$ | $\delta_{\text{c}}$ | $\delta_{\text{t}}$ | $\delta_{\text{c}}$ | $\delta_{\text{t}}$ |
| 0    | 2.624               | 2.183               | 2.625               | 2.183               | 2.625               | 2.184               | 2.625               | 2.186               | 2.625               | 2.186               |
| 1    | 2.607               | 2.151               | 2.605               | 2.149               | 2.603               | 2.147               | 2.601               | 2.147               | 2.599               | 2.147               |
| 2    | 2.575               | 2.110               | 2.571               | 2.108               | 2.567               | 2.107               | 2.564               | 2.107               | 2.562               | 2.107               |
| 3    | 2.536               | 2.078               | 2.533               | 2.078               | 2.529               | 2.078               | 2.526               | 2.078               | 2.524               | 2.079               |
| 4    | 2.497               | 2.056               | 2.493               | 2.055               | 2.488               | 2.055               | 2.486               | 2.055               | 2.483               | 2.055               |
| 5    | 2.435               | 2.032               | 2.434               | 2.033               | 2.433               | 2.033               | 2.432               | 2.034               | 2.430               | 2.034               |
| 6    | 2.399               | 2.023               | 2.396               | 2.023               | 2.395               | 2.023               | 2.395               | 2.023               | 2.395               | 2.023               |

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**Table S5.**  $^1\text{H}$  NMR Chemical Shifts of H2 in Titrations of Mixtures of Stereoisomeric 2-Decalylamines (**3**) with DCl in 3:1  $\text{CD}_3\text{OD}/\text{D}_2\text{O}$  at 25° C.

| titr | mixture of <i>cis</i> and <i>trans</i> stereoisomers |                      |                      |                      | mixture of <i>cis</i> stereoisomers |                      | mixture of <i>trans</i> stereoisomers |                      |
|------|------------------------------------------------------|----------------------|----------------------|----------------------|-------------------------------------|----------------------|---------------------------------------|----------------------|
|      | $\delta_{\text{cc}}$                                 | $\delta_{\text{ct}}$ | $\delta_{\text{tc}}$ | $\delta_{\text{tt}}$ | $\delta_{\text{cc}}$                | $\delta_{\text{ct}}$ | $\delta_{\text{tc}}$                  | $\delta_{\text{tt}}$ |
| -1   | 2.612                                                | 2.795                | 2.627                | 3.129                | 2.611                               | 2.794                | 2.627                                 | 3.130                |
| 0    | 2.620                                                | 2.802                | 2.635                | 3.134                | 2.621                               | 2.803                | 2.636                                 | 3.135                |
| 1    | 2.653                                                | 2.832                | 2.668                | 3.157                | 2.680                               | 2.857                | 2.689                                 | 3.175                |
| 2    | 2.697                                                | 2.872                | 2.704                | 3.185                | 2.736                               | 2.909                | 2.734                                 | 3.211                |
| 3    | 2.724                                                | 2.899                | 2.729                | 3.205                | 2.799                               | 2.968                | 2.778                                 | 3.246                |
| 4    | 2.772                                                | 2.944                | 2.778                | 3.243                | 2.852                               | 3.018                | 2.817                                 | 3.279                |
| 5    | 2.817                                                | 2.988                | 2.820                | 3.281                | 2.915                               | 3.079                | 2.846                                 | 3.303                |
| 6    | 2.852                                                | 3.019                | 2.852                | 3.309                | 2.978                               | 3.138                | 2.888                                 | 3.341                |
| 7    | 2.901                                                | 3.066                | 2.901                | 3.352                | 3.026                               | 3.185                | 2.939                                 | 3.388                |
| 8    | 2.961                                                | 3.122                | 2.961                | 3.409                | 3.083                               | 3.240                | 2.979                                 | 3.427                |
| 9    | 3.002                                                | 3.165                | 3.007                | 3.456                | 3.135                               | 3.291                | 3.031                                 | 3.482                |
| 10   | 3.069                                                | 3.227                | 3.071                | 3.522                |                                     |                      | 3.070                                 | 3.522                |
| 11   | 3.118                                                | 3.276                | 3.126                | 3.581                |                                     |                      | 3.123                                 | 3.581                |
| 12   | 3.137                                                | 3.294                | 3.145                | 3.607                |                                     |                      | 3.144                                 | 3.605                |

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**Table S6.** <sup>1</sup>H NMR Chemical Shifts in Titrations of *trans*-2-Decalylamines (**3<sub>tt</sub>**, **3<sub>tc</sub>**) (H2) with Isopropylamine (**4**) (H2) and with 4-*t*-Butylcyclohexylamine (**1**) (H1) with DCl in 3:1 CD<sub>3</sub>OD/D<sub>2</sub>O at 25° C.

| titr | mixture of <i>trans</i> stereoisomers<br>( <b>3<sub>tc</sub></b> , <b>3<sub>tt</sub></b> ) with isopropyl amine ( <b>4</b> ) |                 |                  | mixture of <i>trans</i> stereoisomers ( <b>3<sub>tc</sub></b> , <b>3<sub>tt</sub></b> )<br>with 4- <i>t</i> -butylcyclohexylamine ( <b>1</b> ) |                 |                |                |
|------|------------------------------------------------------------------------------------------------------------------------------|-----------------|------------------|------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|----------------|----------------|
|      | δ <sub>tc</sub>                                                                                                              | δ <sub>tt</sub> | δ <sub>ipa</sub> | δ <sub>tt</sub>                                                                                                                                | δ <sub>tc</sub> | δ <sub>c</sub> | δ <sub>t</sub> |
| -1   | 2.627                                                                                                                        | 3.129           | 3.045            | 3.129                                                                                                                                          | 2.627           | 2.517          | 3.058          |
| 0    | 2.632                                                                                                                        | 3.133           | 3.050            | 3.135                                                                                                                                          | 2.635           | 2.524          | 3.063          |
| 1    | 2.665                                                                                                                        | 3.157           | 3.083            | 3.169                                                                                                                                          | 2.681           | 2.569          | 3.095          |
| 2    | 2.699                                                                                                                        | 3.183           | 3.116            | 3.195                                                                                                                                          | 2.715           | 2.603          | 3.119          |
| 3    | 2.742                                                                                                                        | 3.216           | 3.155            | 3.227                                                                                                                                          | 2.755           | 2.643          | 3.151          |
| 4    | 2.782                                                                                                                        | 3.249           | 3.192            | 3.261                                                                                                                                          | 2.797           | 2.685          | 3.184          |
| 5    | 2.821                                                                                                                        | 3.282           | 3.224            | 3.295                                                                                                                                          | 2.836           | 2.724          | 3.217          |
| 6    | 2.862                                                                                                                        | <sup>a</sup>    | 3.258            | 3.347                                                                                                                                          | 2.895           | 2.783          | 3.269          |
| 7    | 2.913                                                                                                                        | 3.365           | 3.298            | 3.384                                                                                                                                          | 2.934           | 2.822          | 3.305          |
| 8    | 2.962                                                                                                                        | 3.410           | 3.335            | 3.429                                                                                                                                          | 2.980           | 2.869          | 3.350          |
| 9    | 3.010                                                                                                                        | 3.458           | 3.370            | 3.478                                                                                                                                          | 3.028           | 2.919          | 3.400          |
| 10   | 3.070                                                                                                                        | 3.521           | 3.411            | 3.529                                                                                                                                          | 3.076           | 2.969          | 3.454          |
| 11   | 3.107                                                                                                                        | 3.561           | 3.437            | 3.577                                                                                                                                          | 3.119           | 3.013          | 3.505          |
| 12   | 3.146                                                                                                                        | 3.607           | 3.463            | 3.607                                                                                                                                          | 3.146           | 3.040          | 3.537          |

<sup>a</sup> Interference from the CD<sub>2</sub>HOD peak.