

## Supplementary data

### *Ab initio* study of chiral recognition in the propylene imine hydrogen peroxide complex

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**Table S1.** Geometrical parameters (Å and degrees) for complexes: (anti) *cis*-PI • *P*-HOOH [***cis*I**], (anti) *cis*-PI • *M*-HOOH [***cis*I'**], (syn) *cis*-PI • *P*-HOOH [***cis*II**], (syn) *cis*-PI • *M*-HOOH [***cis*II'**], (syn) *trans*-PI • *P*-HOOH [***trans*I**], (syn) *trans*-PI • *M*-HOOH [***trans*I'**], (anti) *trans*-PI • *P*-HOOH [***trans*II**], (anti) *trans*-PI • *M*-HOOH [***trans*II'**], and PI and HOOH monomers using MP2/aug-cc-pVDZ.

|  | <i>cisI</i> | <i>cisI'</i> | <i>cisII</i> | <i>cisII'</i> | <i>cis-PI</i> | <i>transI</i> | <i>transI'</i> | <i>transII</i> | <i>transII'</i> | <i>trans-PI</i> | <i>P/M-HOOH</i> |
|--|-------------|--------------|--------------|---------------|---------------|---------------|----------------|----------------|-----------------|-----------------|-----------------|
| N <sub>1</sub> -C <sub>2</sub>                                       | 1.498       | 1.499        | 1.494        | 1.497         | 1.497         | 1.497         | 1.495          | 1.494          | 1.494           | 1.496           | –               |
| N <sub>1</sub> -C <sub>3</sub>                                       | 1.491       | 1.490        | 1.486        | 1.487         | 1.487         | 1.493         | 1.490          | 1.486          | 1.487           | 1.489           | –               |
| N <sub>1</sub> -H <sub>5</sub>                                       | 1.023       | 1.023        | 1.025        | 1.026         | 1.025         | 1.022         | 1.022          | 1.024          | 1.024           | 1.024           | –               |
| C <sub>2</sub> -C <sub>3</sub>                                       | 1.489       | 1.489        | 1.491        | 1.491         | 1.490         | 1.491         | 1.492          | 1.491          | 1.491           | 1.491           | –               |
| C <sub>2</sub> -H <sub>6</sub>                                       | 1.090       | 1.091        | 1.092        | 1.092         | 1.092         | 1.092         | 1.092          | 1.093          | 1.092           | 1.093           | –               |
| C <sub>2</sub> -H <sub>7</sub>                                       | 1.093       | 1.093        | 1.094        | 1.094         | 1.094         | 1.092         | 1.092          | 1.093          | 1.093           | 1.093           | –               |
| C <sub>3</sub> -C <sub>4</sub>                                       | 1.510       | 1.510        | 1.512        | 1.512         | 1.511         | 1.510         | 1.510          | 1.510          | 1.510           | 1.510           | –               |
| C <sub>3</sub> -H <sub>8</sub>                                       | 1.094       | 1.093        | 1.095        | 1.095         | 1.095         | 1.095         | 1.095          | 1.095          | 1.095           | 1.096           | –               |
| C <sub>4</sub> -H <sub>9</sub>                                       | 1.103       | 1.103        | 1.101        | 1.102         | 1.103         | 1.100         | 1.101          | 1.10           | 1.101           | 1.101           | –               |
| C <sub>4</sub> -H <sub>10</sub>                                      | 1.102       | 1.102        | 1.103        | 1.102         | 1.102         | 1.100         | 1.101          | 1.102          | 1.102           | 1.102           | –               |
| C <sub>4</sub> -H <sub>11</sub>                                      | 1.102       | 1.102        | 1.103        | 1.103         | 1.102         | 1.102         | 1.102          | 1.103          | 1.103           | 1.102           | –               |
| □ C <sub>2</sub> -N <sub>1</sub> -H <sub>5</sub>                     | 109.5       | 109.5        | 107.6        | 107.4         | 108.1         | 109.8         | 110.0          | 107.9          | 107.7           | 108.4           | –               |
| □ C <sub>3</sub> -N <sub>1</sub> -H <sub>5</sub>                     | 109.4       | 109.5        | 107.6        | 107.4         | 108.0         | 110.4         | 110.4          | 108.4          | 108.3           | 109.2           | –               |
| □ N <sub>1</sub> -C <sub>3</sub> -C <sub>4</sub>                     | 119.1       | 118.9        | 119.5        | 119.1         | 119.6         | 116.0         | 115.6          | 115.7          | 115.5           | 115.3           | –               |
| □ C <sub>2</sub> -C <sub>3</sub> -C <sub>4</sub>                     | 120.7       | 120.5        | 120.1        | 119.9         | 120.3         | 121.2         | 121.1          | 121.3          | 121.1           | 121.1           | –               |
| □ C <sub>4</sub> -C <sub>3</sub> -N <sub>1</sub> -H <sub>5</sub>     | -9.0        | -9.0         | -9.3         | -9.6          | -9.2          | 145.7         | 145.4          | 146.6          | 147.0           | 146.5           | –               |
| O <sub>12</sub> -O <sub>13</sub>                                     | 1.476       | 1.476        | 1.471        | 1.471         | –             | 1.474         | 1.474          | 1.471          | 1.471           | –               | 1.470           |
| O <sub>12</sub> -H <sub>14</sub>                                     | 0.996       | 0.996        | 0.972        | 0.973         | –             | 0.996         | 0.994          | 0.973          | 0.973           | –               | 0.972           |
| O <sub>13</sub> -H <sub>15</sub>                                     | 0.971       | 0.971        | 0.972        | 0.972         | –             | 0.971         | 0.971          | 0.972          | 0.972           | –               | 0.972           |
| □ O <sub>12</sub> -O <sub>13</sub> -H <sub>15</sub>                  | 98.9        | 98.8         | 99.1         | 99.2          | –             | 99.0          | 99.0           | 99.3           | 99.2            | –               | 99.1            |
| □ O <sub>13</sub> -O <sub>12</sub> -H <sub>14</sub>                  | 97.9        | 97.9         | 99.3         | 99.4          | –             | 98.9          | 98.6           | 99.1           | 99.4            | –               | 99.1            |
| □ H <sub>14</sub> -O <sub>12</sub> -O <sub>13</sub> -H <sub>15</sub> | 116.8       | -117.4       | 114.5        | -112.4        | –             | 113.3         | -114.3         | 112.2          | -112.2          | –               | +/-112.9        |

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|  |       |       |       |       |   |       |       |       |       |   |   |
|--|-------|-------|-------|-------|---|-------|-------|-------|-------|---|---|
| N <sub>1</sub> ...H <sub>14</sub>                    | 1.772 | 1.772 | –     | –     | – | 1.767 | 1.777 | –     | –     | – | – |
| H <sub>5</sub> ...O <sub>12</sub>                    | –     | –     | 2.225 | 2.258 | – | –     | –     | 2.218 | 2.243 | – | – |
| □ N <sub>1</sub> ...H <sub>14</sub> -O <sub>12</sub> | 164.3 | 164.9 | –     | –     | – | 169.5 | 176.5 | –     | –     | – | – |
| □ N <sub>1</sub> -H <sub>5</sub> ...O <sub>12</sub>  | –     | –     | 177.7 | 152.3 | – | –     | –     | 168.7 | 163.2 | – | – |

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