

## ELECTRONIC SUPPLEMENTARY INFORMATION

### High-level analytical potential-energy-surface-based dynamics of the $\text{OH}^- + \text{CH}_3\text{CH}_2\text{Cl}$ $\text{S}_{\text{N}}2$ and $\text{E}2$ reactions in full (24) dimensions

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**Table S1.** Harmonic vibrational frequencies (in  $\text{cm}^{-1}$ ) of the reactants and products of the  $\text{OH}^- + \text{CH}_3\text{CH}_2\text{Cl}$  reaction corresponding to the analytical PES.

| Nr. | $\text{CH}_3\text{CH}_2\text{Cl}$ | $\text{OH}^-$ | $\text{CH}_3\text{CH}_2\text{OH}$ | $\text{C}_2\text{H}_4$ | $\text{H}_2\text{O}$ | $\text{CH}_3\text{CHCl}^-$ | $\text{H}_2\text{O}\cdots\text{Cl}^-$ |
|-----|-----------------------------------|---------------|-----------------------------------|------------------------|----------------------|----------------------------|---------------------------------------|
| 1   | 317                               | 3771          | 123                               | 735                    | 1752                 | 103                        | 224                                   |
| 2   | 356                               |               | 268                               | 937                    | 3841                 | 296                        | 393                                   |
| 3   | 747                               |               | 490                               | 944                    | 3930                 | 431                        | 648                                   |
| 4   | 851                               |               | 796                               | 1235                   |                      | 475                        | 1726                                  |
| 5   | 955                               |               | 875                               | 1252                   |                      | 908                        | 3288                                  |
| 6   | 1066                              |               | 1089                              | 1346                   |                      | 1085                       | 3991                                  |
| 7   | 1099                              |               | 1128                              | 1578                   |                      | 1093                       |                                       |
| 8   | 1305                              |               | 1191                              | 1699                   |                      | 1154                       |                                       |
| 9   | 1315                              |               | 1236                              | 2971                   |                      | 1265                       |                                       |
| 10  | 1395                              |               | 1326                              | 3057                   |                      | 1369                       |                                       |
| 11  | 1513                              |               | 1374                              | 3126                   |                      | 1517                       |                                       |
| 12  | 1523                              |               | 1444                              | 3238                   |                      | 1611                       |                                       |
| 13  | 1571                              |               | 1481                              |                        |                      | 1724                       |                                       |
| 14  | 2987                              |               | 1530                              |                        |                      | 2762                       |                                       |
| 15  | 3038                              |               | 1589                              |                        |                      | 2979                       |                                       |
| 16  | 3189                              |               | 2961                              |                        |                      | 3026                       |                                       |
| 17  | 3233                              |               | 3001                              |                        |                      | 3279                       |                                       |
| 18  | 3312                              |               | 3021                              |                        |                      | 3698                       |                                       |
| 19  |                                   |               | 3152                              |                        |                      |                            |                                       |
| 20  |                                   |               | 3194                              |                        |                      |                            |                                       |
| 21  |                                   |               | 3864                              |                        |                      |                            |                                       |

**Table S2.** Cross sections (in bohr<sup>2</sup>) of the various pathways of the OH<sup>-</sup> + CH<sub>3</sub>CH<sub>2</sub>Cl reaction at different collision energies.

| <i>E</i> <sub>coll</sub> (kcal/mol) | S <sub>N</sub> 2 Unrestricted | S <sub>N</sub> 2 Soft restricted | S <sub>N</sub> 2 Hard restricted | S <sub>N</sub> 2 (H-exchange)      |
|-------------------------------------|-------------------------------|----------------------------------|----------------------------------|------------------------------------|
| 1                                   | 177.33                        | 204.19                           | 304.72                           | 12.84                              |
| 5                                   | 70.16                         | 76.91                            | 100.22                           | 3.73                               |
| 10                                  | 23.18                         | 24.25                            | 27.92                            | 1.17                               |
| 20                                  | 4.67                          | 4.82                             | 5.14                             | 0.15                               |
| 30                                  | 2.47                          | 2.48                             | 2.58                             | 0.06                               |
| 40                                  | 2.33                          | 2.35                             | 2.43                             | 0.01                               |
| 50                                  | 2.66                          | 2.68                             | 2.76                             | 0.00                               |
| <i>E</i> <sub>coll</sub> (kcal/mol) | H-Abs Unrestricted            | H-Abs Soft restricted            | H-Abs Hard restricted            | H <sub>2</sub> O...Cl <sup>-</sup> |
| 1                                   | 19.56                         | 0.00                             | 0.00                             | 7.78                               |
| 5                                   | 22.26                         | 0.00                             | 0.00                             | 4.59                               |
| 10                                  | 12.98                         | 0.00                             | 0.00                             | 3.97                               |
| 20                                  | 7.55                          | 0.38                             | 0.04                             | 1.93                               |
| 30                                  | 5.88                          | 1.22                             | 0.29                             | 0.67                               |
| 40                                  | 5.39                          | 1.55                             | 0.53                             | 0.51                               |
| 50                                  | 4.78                          | 1.51                             | 0.55                             | 0.36                               |
| <i>E</i> <sub>coll</sub> (kcal/mol) | E2 Unrestricted               | E2 Soft restricted               | E2 Hard restricted               | E2 (H-exchange)                    |
| 1                                   | 873.59                        | 791.31                           | 485.09                           | 27.01                              |
| 5                                   | 339.66                        | 311.16                           | 182.51                           | 9.05                               |
| 10                                  | 118.06                        | 107.46                           | 60.39                            | 2.49                               |
| 20                                  | 31.58                         | 29.28                            | 16.18                            | 0.38                               |
| 30                                  | 17.29                         | 16.22                            | 9.21                             | 0.16                               |
| 40                                  | 13.40                         | 12.52                            | 7.34                             | 0.06                               |
| 50                                  | 11.17                         | 10.60                            | 5.89                             | 0.02                               |
| <i>E</i> <sub>coll</sub> (kcal/mol) | <i>anti</i> -E2               | <i>syn</i> -E2                   | Induced inversion                | H-exchange                         |
| 1                                   | 862.47                        | 11.12                            | 0.51                             | 6.93                               |
| 5                                   | 331.82                        | 7.84                             | 0.13                             | 4.78                               |
| 10                                  | 112.55                        | 5.50                             | 0.08                             | 1.75                               |
| 20                                  | 27.09                         | 4.49                             | 0.01                             | 0.31                               |
| 30                                  | 13.48                         | 3.80                             | 0.01                             | 0.08                               |
| 40                                  | 9.84                          | 3.56                             | 0.00                             | 0.02                               |
| 50                                  | 7.75                          | 3.41                             | 0.00                             | 0.00                               |