# Supporting Information

Table S1: B3LYP/6-311G(d,p) optimized geometry of (*S*)-methyloxirane (in a.u.)

| | x | y | z |
|---|---|---|---|
| C | 0.28658573 | -0.06842314 | 0.923615545 |
| C | -1.97167357 | 1.16281695 | -0.11611594 |
| O | -1.56077904 | -1.49136505 | -0.45642963 |
| H | -1.79951788 | 2.30301858 | -1.81860990 |
| H | -3.53368130 | 1.66205020 | 1.12314027 |
| H | 0.28935676 | -0.47792278 | 2.94204590 |
| C | 2.85182915 | 0.18852554 | -0.28024045 |
| H | 2.67061628 | 0.61324913 | -2.29190002 |
| H | 3.93617089 | 1.70148365 | 0.62084953 |
| H | 3.92283966 | -1.56847438 | -0.08764369 |

Table S2: B3LYP/6-311G(d,p) optimized geometry of (*1S*,*4S*)-norbornenone (in a.u.)

| | x | y | z |
|---|---|---|---|
| C | 2.22029782 | -0.00675010 | -0.07807404 |
| C | -1.51317363 | -2.43829473 | -0.98195461 |
| C | 0.21881895 | -1.71011144 | 1.21188326 |
| C | 0.80312983 | 2.44015233 | -0.79730191 |
| C | -1.94579053 | 1.80021359 | 0.02972161 |
| C | -2.80142073 | -0.37577204 | -1.66521155 |
| H | -1.48641133 | -4.26059355 | -1.90791286 |
| H | 1.02414086 | -3.23370314 | 2.33012492 |
| H | 1.01435774 | 2.87458714 | -2.80077822 |
| H | 1.60616706 | 4.00919383 | 0.28560376 |
| H | -3.21336213 | 3.41639997 | 0.15659971 |
| H | -4.07376388 | -0.18626086 | -3.25568065 |
| O | 4.41271272 | -0.48272676 | -0.43476173 |
| C | -1.42269166 | 0.33260692 | 2.51323938 |
| H | -3.12946207 | -0.46044878 | 3.35642762 |
| H | -0.39838639 | 1.45035347 | 3.91989482 |

Table S3: B3LYP/6-311G(d,p) optimized geometry of (*S*)-2-chloropropionitrile (in a.u.)

| | x | y | z |
|---|---|---|---|
| C | -0.06317921 | 0.67368170 | 0.82832744 |
| C | -2.43926227 | -0.56030191 | 0.17303466 |
| N | -4.35328083 | -1.46760478 | -0.33151277 |
| H | 0.08607892 | 0.75994014 | 2.88076844 |
| Cl | 2.56743673 | -1.34149957 | -0.15816819 |
| C | 0.17726009 | 3.30015914 | -0.33937025 |
| H | 1.96416056 | 4.15306624 | 0.22950346 |
| H | -1.37546551 | 4.49066392 | 0.32254790 |
| H | 0.10286913 | 3.19381858 | -2.39532425 |

The values utilized in this work for the regular, cubic grids are summarized by Table S5. For the multigrid solver, both the error tolerance and the defect correction error tolerance were set to $1 \times 10^{-7}$. For the Gaussian functions used to represent the nuclear density, the smearing width was set to 0.25 $a_0$. For the two parameters used to defined the dielectric permittivity, the most accurate parameterization of $\beta = 1.6$ and $\rho_0 = 0.00055$ (based on r.m.s. from experiment) was chosen [Dziedzic *et al.* EPL,**95** (2011) 43001].

Table S4: Summary of grid sizes utilized in calculations. The number of grid points in each of the x, y and z directions (npts) and the spacing between grid points (in a.u.) are given for each molecule

| | npts | $\Delta$h |
|---|---|---|
| (*S*)-methyloxirane | 609 | 0.057 |
| (*1S,4S*)-norbornenone | 641 | 0.053 |
| 2-(*S*)-chloropropionitrile | 769 | 0.0515 |

Table S5: Dielectric constants of solvents used in this work

| | |
|---|---|
| Water | 78.54 |
| Acetonitrile | 35.69 |
| Ethanol | 24.85 |
| Cyclohexane | 2.02 |
| Carbon tetrachloride | 2.23 |
| Benzene | 2.27 |
| Dibutyl Ether | 3.05 |
| Methanol | 32.61 |