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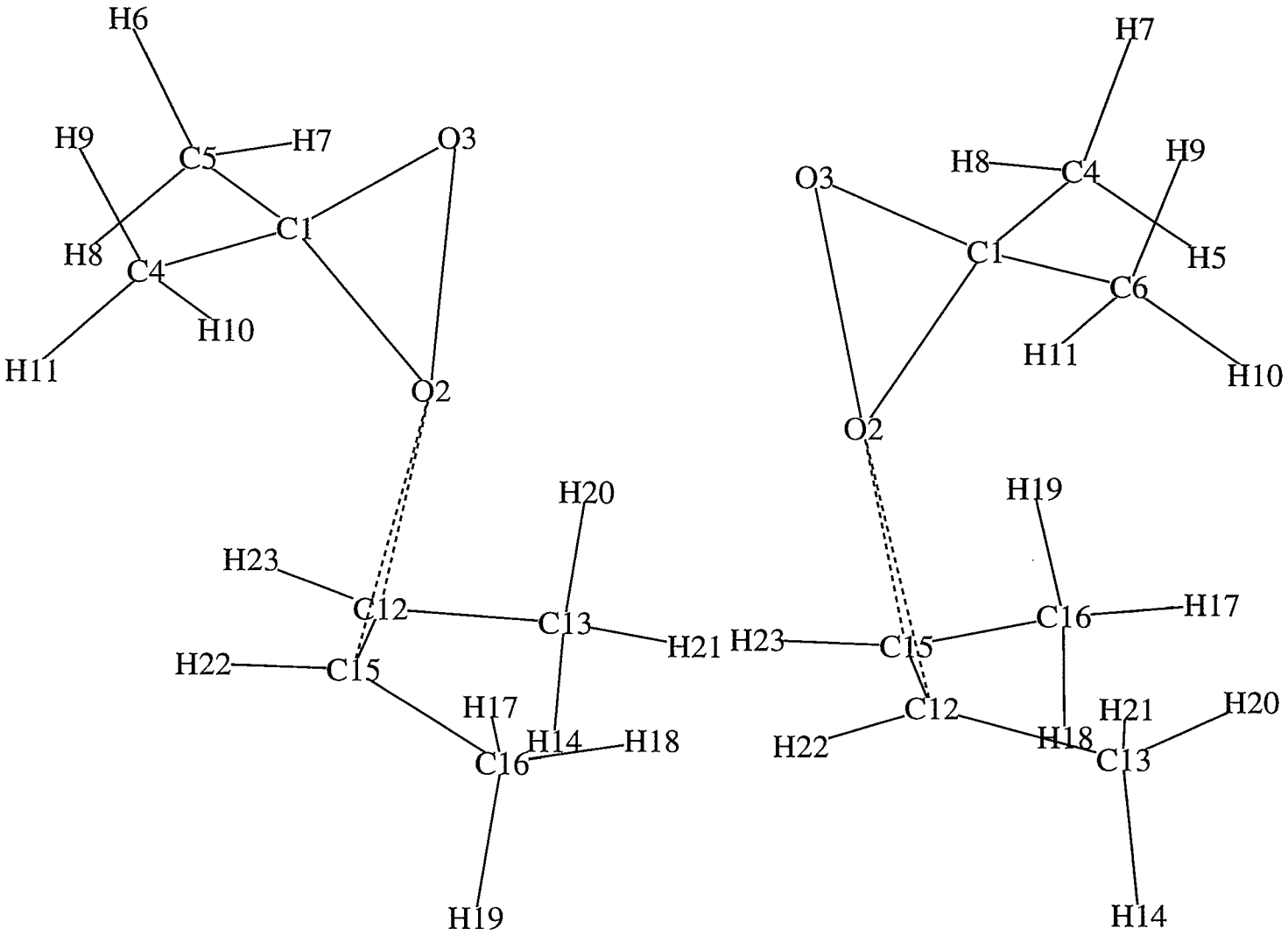

Supplementary Figure 1. Numbering Scheme for *Anti* (left) and *Syn* (right) Systems

Supplementary Table 1a. Non-Bonded Parameters for *Anti* Reactants

Atom	q (e)	σ (Å)	ε (kcal/mol)
C1	0.6623	3.50	0.066
O2	-0.2576	2.90	0.140
O3	-0.2576	2.90	0.140
C4	-0.3654	3.50	0.066
C5	-0.3654	3.50	0.066
H6	0.0970	2.50	0.030
H7	0.0979	2.50	0.030
H8	0.0970	2.50	0.030
H9	0.0970	2.50	0.030
H10	0.0979	2.50	0.030
H11	0.0970	2.50	0.030
C12	-0.1856	3.55	0.076
C13	0.1015	3.50	0.066
H14	-0.0056	2.50	0.030
C15	-0.1856	3.55	0.076
C16	0.1018	3.50	0.066
H17	-0.0057	2.50	0.030
H18	0.0024	2.50	0.030
H19	-0.0058	2.50	0.030
H20	-0.0057	2.50	0.030
H21	0.0024	2.50	0.030
H22	0.0929	2.42	0.030
H23	0.0929	2.42	0.030

Supplementary Table 1b. Non-Bonded Parameters for *Anti* Transition Structure

Atom	q (e)	σ (Å)	ε (kcal/mol)
C1	0.7983	3.50	0.066
O2	-0.3259	2.90	0.140
O3	-0.5171	2.90	0.140
C4	-0.3738	3.50	0.066
C5	-0.3742	3.50	0.066
H6	0.0842	2.50	0.030
H7	0.0920	2.50	0.030
H8	0.0598	2.50	0.030
H9	0.0840	2.50	0.030
H10	0.0920	2.50	0.030
H11	0.0598	2.50	0.030
C12	0.0040	3.55	0.076
C13	-0.0784	3.50	0.066
H14	0.0348	2.50	0.030
C15	0.0050	3.55	0.076
C16	-0.0796	3.50	0.066
H17	0.0601	2.50	0.030
H18	0.0634	2.50	0.030
H19	0.0349	2.50	0.030
H20	0.0598	2.50	0.030
H21	0.0629	2.50	0.030
H22	0.0769	2.42	0.030
H23	0.0771	2.42	0.030

Supplementary Table 1c. Non-Bonded Parameters for *Syn* Reactants

Atom	q (e)	σ (Å)	ε (kcal/mol)
C1	0.6623	3.50	0.066
O2	-0.2577	2.90	0.140
O3	-0.2577	2.90	0.140
C4	-0.3654	3.50	0.066
H5	0.0970	2.50	0.030
C6	-0.3654	3.50	0.066
H7	0.0970	2.50	0.030
H8	0.0979	2.50	0.030
H9	0.0970	2.50	0.030
H10	0.0970	2.50	0.030
H11	0.0979	2.50	0.030
C12	-0.1855	3.55	0.076
C13	0.1015	3.50	0.066
H14	-0.0057	2.50	0.030
C15	-0.1855	3.55	0.076
C16	0.1018	3.50	0.066
H17	0.0024	2.50	0.030
H18	-0.0057	2.50	0.030
H19	-0.0058	2.50	0.030
H20	0.0024	2.50	0.030
H21	-0.0056	2.50	0.030
H22	0.0929	2.42	0.030
H23	0.0929	2.42	0.030

Supplementary Table 1d. Non-Bonded Parameters for *Syn* Transition Structure

Atom	q (e)	σ (Å)	ε (kcal/mol)
C1	0.8165	3.50	0.066
O2	-0.3516	2.90	0.140
O3	-0.5249	2.90	0.140
C4	-0.3325	3.50	0.066
H5	0.0429	2.50	0.030
C6	-0.3320	3.50	0.066
H7	0.0702	2.50	0.030
H8	0.0785	2.50	0.030
H9	0.0702	2.50	0.030
H10	0.0426	2.50	0.030
H11	0.0784	2.50	0.030
C12	0.0014	3.55	0.076
C13	-0.0513	3.50	0.066
H14	0.0279	2.50	0.030
C15	0.0002	3.55	0.076
C16	-0.0513	3.50	0.066
H17	0.0460	2.50	0.030
H18	0.0281	2.50	0.030
H19	0.0515	2.50	0.030
H20	0.0465	2.50	0.030
H21	0.0514	2.50	0.030
H22	0.0955	2.42	0.030
H23	0.0958	2.42	0.030

Structure of dimethyldioxirane in PDB format is given below:

```
HEADER
REMARK dimethyldioxirane E = -268.268901 au
HETATM    1  C   UNK     1      -0.374   0.258   0.052  0.00  0.00    0
HETATM    2  O   UNK     1      -1.683   0.544  -0.367  0.00  0.00    0
HETATM    3  O   UNK     1      -1.003   1.307   0.738  0.00  0.00    0
HETATM    4  C   UNK     1       0.723   0.663  -0.903  0.00  0.00    0
HETATM    5  H   UNK     1       0.870  -0.109  -1.666  0.00  0.00    0
HETATM    6  H   UNK     1       0.456   1.604  -1.388  0.00  0.00    0
HETATM    7  H   UNK     1       1.670   0.790  -0.365  0.00  0.00    0
HETATM    8  C   UNK     1      -0.199  -1.024   0.830  0.00  0.00    0
HETATM    9  H   UNK     1      -1.068  -1.182   1.473  0.00  0.00    0
HETATM   10  H   UNK     1      -0.095  -1.874   0.147  0.00  0.00    0
HETATM   11  H   UNK     1       0.704  -0.975   1.448  0.00  0.00    0
END
```

Structure of *cis*-2-butene in PDB format is given below:

```
HEADER
REMARK cis-2-butene E = -157.2247548 au
HETATM    1  C   UNK     1      -0.669   0.783   0.000  0.00  0.00    0
HETATM    2  C   UNK     1       0.669   0.783   0.000  0.00  0.00    0
HETATM    3  H   UNK     1      -1.170   1.752   0.000  0.00  0.00    0
HETATM    4  H   UNK     1       1.170   1.752   0.000  0.00  0.00    0
HETATM    5  C   UNK     1      -1.593  -0.403   0.000  0.00  0.00    0
HETATM    6  H   UNK     1      -2.252  -0.386  -0.879  0.00  0.00    0
HETATM    7  H   UNK     1      -1.061  -1.358  -0.001  0.00  0.00    0
HETATM    8  H   UNK     1      -2.250  -0.387   0.881  0.00  0.00    0
HETATM    9  C   UNK     1       1.593  -0.403   0.000  0.00  0.00    0
HETATM   10  H   UNK     1       2.251  -0.386   0.880  0.00  0.00    0
HETATM   11  H   UNK     1       1.061  -1.358   0.001  0.00  0.00    0
HETATM   12  H   UNK     1       2.250  -0.387  -0.880  0.00  0.00    0
END
```

Structure of *trans*-2-butene in PDB format is given below:

```
HEADER
REMARK trans-2-butene E = -157.2269605 au
HETATM    1  C   UNK     1       0.477  -0.443   0.148  0.00  0.00    0
HETATM    2  C   UNK     1      -0.477   0.443  -0.148  0.00  0.00    0
HETATM    3  H   UNK     1      -0.193   1.372  -0.648  0.00  0.00    0
HETATM    4  H   UNK     1       0.193  -1.372   0.647  0.00  0.00    0
HETATM    5  C   UNK     1       1.940  -0.275  -0.150  0.00  0.00    0
HETATM    6  H   UNK     1       2.142   0.679  -0.649  0.00  0.00    0
HETATM    7  H   UNK     1       2.542  -0.310   0.769  0.00  0.00    0
HETATM    8  H   UNK     1       2.311  -1.082  -0.797  0.00  0.00    0
HETATM    9  C   UNK     1      -1.940   0.275   0.150  0.00  0.00    0
HETATM   10  H   UNK     1      -2.142  -0.679   0.649  0.00  0.00    0
HETATM   11  H   UNK     1      -2.311   1.082   0.797  0.00  0.00    0
HETATM   12  H   UNK     1      -2.542   0.310  -0.769  0.00  0.00    0
END
```

Structure of the *anti* transition structure for DMD and *cis*-2-butene in PDB format is given below:

```
HEADER
REMARK anti TS cis-2-butene B3LYP/6-31G*//B3LYP/6-31G* E = -425.4715864 au
HETATM    1  C   UNK     1       0.822   1.525   0.096  0.00  0.00    0
HETATM    2  O   UNK     1      -0.049   2.485   0.378  0.00  0.00    0
HETATM    3  O   UNK     1      -0.373   0.642   0.155  0.00  0.00    0
HETATM    4  C   UNK     1      -0.336  -1.343   0.560  0.00  0.00    0
HETATM    5  C   UNK     1      -0.552  -1.141  -0.788  0.00  0.00    0
HETATM    6  H   UNK     1       0.693  -1.496   0.876  0.00  0.00    0
HETATM    7  C   UNK     1      -1.376  -1.525   1.619  0.00  0.00    0
HETATM    8  H   UNK     1      -2.362  -1.180   1.303  0.00  0.00    0
HETATM    9  H   UNK     1      -1.454  -2.587   1.892  0.00  0.00    0
HETATM   10  H   UNK     1      -1.094  -0.975   2.523  0.00  0.00    0
HETATM   11  H   UNK     1       0.323  -1.150  -1.433  0.00  0.00    0
HETATM   12  C   UNK     1      -1.872  -1.060  -1.486  0.00  0.00    0
HETATM   13  H   UNK     1      -2.697  -0.862  -0.799  0.00  0.00    0
HETATM   14  H   UNK     1      -1.855  -0.265  -2.238  0.00  0.00    0
HETATM   15  H   UNK     1      -2.080  -2.004  -2.010  0.00  0.00    0
HETATM   16  C   UNK     1       1.830   1.194   1.198  0.00  0.00    0
HETATM   17  H   UNK     1       2.559   2.009   1.272  0.00  0.00    0
HETATM   18  H   UNK     1       1.306   1.113   2.154  0.00  0.00    0
HETATM   19  H   UNK     1       2.385   0.269   1.001  0.00  0.00    0
HETATM   20  C   UNK     1       1.430   1.566  -1.307  0.00  0.00    0
HETATM   21  H   UNK     1       0.637   1.737  -2.039  0.00  0.00    0
HETATM   22  H   UNK     1       2.139   2.400  -1.365  0.00  0.00    0
HETATM   23  H   UNK     1       1.975   0.648  -1.560  0.00  0.00    0
END
```

Structure of the *syn* transition structure for DMD and *cis*-2-butene in PDB format is given below:

```
HEADER
REMARK syn TS cis-2-butene B3LYP/6-31G*//B3LYP/6-31G* E = -425.4662337 au
HETATM    1  C   UNK     1       0.822   1.525   0.096  0.00  0.00    0
HETATM    2  O   UNK     1      -0.049   2.485   0.378  0.00  0.00    0
HETATM    3  O   UNK     1      -0.373   0.642   0.155  0.00  0.00    0
HETATM    4  C   UNK     1      -0.336  -1.343   0.560  0.00  0.00    0
HETATM    5  C   UNK     1      -0.552  -1.141  -0.788  0.00  0.00    0
HETATM    6  H   UNK     1       0.693  -1.496   0.876  0.00  0.00    0
HETATM    7  C   UNK     1      -1.376  -1.525   1.619  0.00  0.00    0
HETATM    8  H   UNK     1      -2.362  -1.180   1.303  0.00  0.00    0
HETATM    9  H   UNK     1      -1.454  -2.587   1.892  0.00  0.00    0
HETATM   10  H   UNK     1      -1.094  -0.975   2.523  0.00  0.00    0
HETATM   11  H   UNK     1       0.323  -1.150  -1.433  0.00  0.00    0
HETATM   12  C   UNK     1      -1.872  -1.060  -1.486  0.00  0.00    0
HETATM   13  H   UNK     1      -2.697  -0.862  -0.799  0.00  0.00    0
HETATM   14  H   UNK     1      -1.855  -0.265  -2.238  0.00  0.00    0
HETATM   15  H   UNK     1      -2.080  -2.004  -2.010  0.00  0.00    0
HETATM   16  C   UNK     1       1.830   1.194   1.198  0.00  0.00    0
HETATM   17  H   UNK     1       2.559   2.009   1.272  0.00  0.00    0
HETATM   18  H   UNK     1       1.306   1.113   2.154  0.00  0.00    0
HETATM   19  H   UNK     1       2.385   0.269   1.001  0.00  0.00    0
HETATM   20  C   UNK     1       1.430   1.566  -1.307  0.00  0.00    0
HETATM   21  H   UNK     1       0.637   1.737  -2.039  0.00  0.00    0
HETATM   22  H   UNK     1       2.139   2.400  -1.365  0.00  0.00    0
HETATM   23  H   UNK     1       1.975   0.648  -1.560  0.00  0.00    0
END
```

Structure of the transition structure for DMD and *trans*-2-butene in PDB format is given below:

```
HEADER
REMARK TS trans-2-butene B3LYP/6-31G*//B3LYP/6-31G* E = -425.4711724 au
HETATM    1  C   UNK     1      -0.274    1.588    0.361  0.00  0.00    0
HETATM    2  O   UNK     1       0.704    2.478    0.274  0.00  0.00    0
HETATM    3  O   UNK     1       0.806    0.615    0.010  0.00  0.00    0
HETATM    4  C   UNK     1       0.601   -1.014   -1.014  0.00  0.00    0
HETATM    5  C   UNK     1       0.831   -1.509    0.251  0.00  0.00    0
HETATM    6  H   UNK     1      -0.430   -0.973   -1.362  0.00  0.00    0
HETATM    7  C   UNK     1       1.664   -0.822   -2.053  0.00  0.00    0
HETATM    8  H   UNK     1       2.654   -0.748   -1.596  0.00  0.00    0
HETATM    9  H   UNK     1       1.667   -1.668   -2.754  0.00  0.00    0
HETATM   10  H   UNK     1       1.481    0.091   -2.627  0.00  0.00    0
HETATM   11  H   UNK     1       1.865   -1.604    0.577  0.00  0.00    0
HETATM   12  C   UNK     1      -1.350    1.665   -0.722  0.00  0.00    0
HETATM   13  H   UNK     1      -1.979    2.544   -0.539  0.00  0.00    0
HETATM   14  H   UNK     1      -0.874    1.782   -1.700  0.00  0.00    0
HETATM   15  H   UNK     1      -2.004    0.785   -0.732  0.00  0.00    0
HETATM   16  C   UNK     1      -0.822    1.353    1.768  0.00  0.00    0
HETATM   17  H   UNK     1       0.013    1.215    2.459  0.00  0.00    0
HETATM   18  H   UNK     1      -1.386    2.240    2.080  0.00  0.00    0
HETATM   19  H   UNK     1      -1.495    0.490    1.823  0.00  0.00    0
HETATM   20  C   UNK     1      -0.218   -2.015    1.185  0.00  0.00    0
HETATM   21  H   UNK     1      -1.229   -1.846    0.802  0.00  0.00    0
HETATM   22  H   UNK     1      -0.090   -3.097    1.335  0.00  0.00    0
HETATM   23  H   UNK     1      -0.134   -1.548    2.173  0.00  0.00    0
END
```

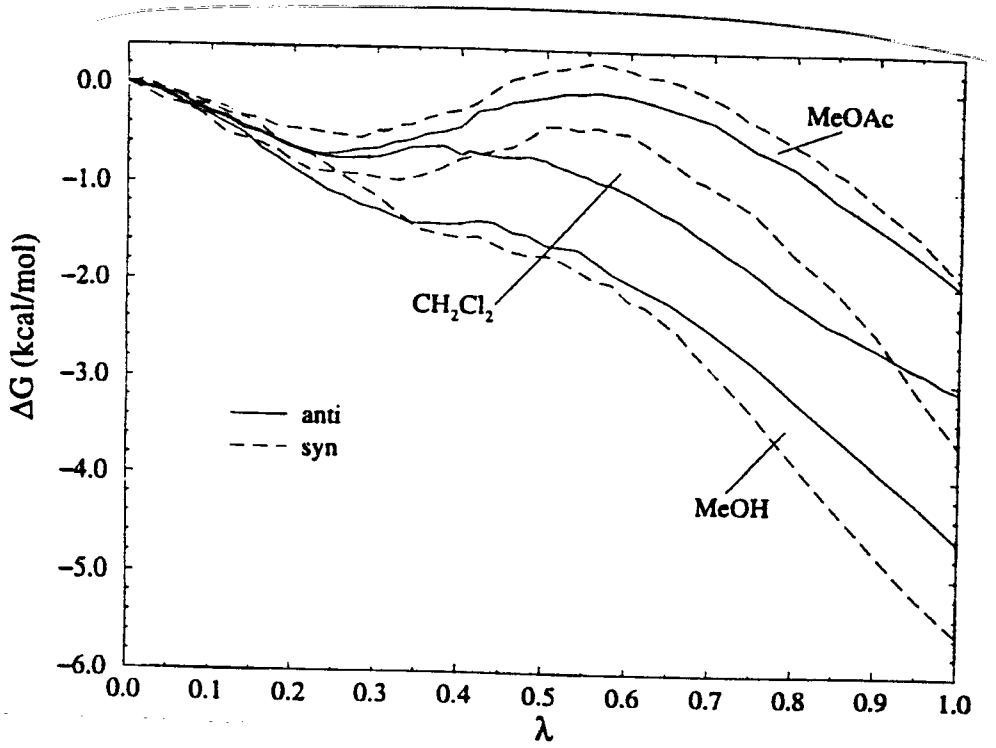

Figure 2. Computed changes in free energies of solvation in CH_3OAc, CH_2Cl_2, and CH_3OH for the epoxidations of *cis*-2-butene leading from the reactants at $l = 0.0$ to the anti and syn transition structures at $\lambda = 1.0$ (λ is the reaction coordinate used in the FEP calculations).