Supporting Information

Water clusters as bifunctional catalysts in organic chemistry. The hydrolysis of oxirane and its methyl derivatives.

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Computational details

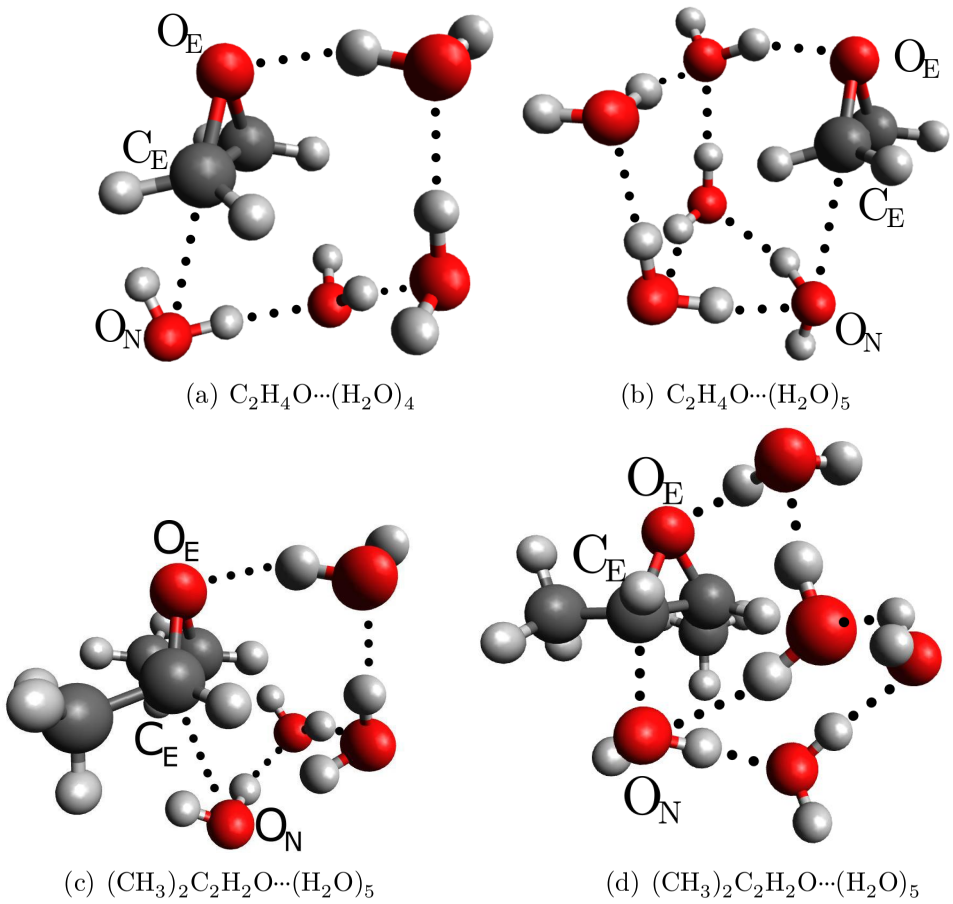
We optimised the geometry of all reactants, products, intermediates and transition states using the M06-2X [1] functional with the 6-311++G(2d,2p) basis set as implemented in the Gaussian 16 package [2]. We chose the M06-2X approximation for such calculations because it is suitable for the description of geometries, kinetics and thermodynamics of H-bonded systems [3]. We used these optimised geometries to carry out single point calculations with the approximation DLNPO-CCSD(T)/aug-cc-pVTZ with the Orca 4.2.1 [4, 5] software to take into account electron correlation effects more accurately than it is done with approximate exchange-correlation functionals. (2.6) The complete specification of the stereochemistry of the chiral epoxides addressed in this research is (i) (R)-2-methyl oxirane, (ii) (2R,3R)-2,3-dimethyl oxirane (trans) and (iii) (3R)-2,2,3-trimethyl oxirane.

We took into account solvent effects in the calculations via the implicit solvent model SMD method (water) [6]. In addition, we performed Intrinsic Reaction Coordinate (IRC) calculations to verify the connection between reactants and products and we characterised each structure as a minimum via the corresponding harmonic frequencies. We performed the calculations considering the following temperatures (i) 298.15 for oxirane, methyl oxirane and 2,2-dimethyl oxirane and (ii) 343.15 K for oxirane. The choice of these temperatures is due to the experimental conditions reported for these reactions along with the corresponding rate constants found in the literature[7].

Given our previous experience of water clusters as bifunctional catalysts in inorganic chemistry [8], we considered only homodromic networks of hydrogen bonds because they present the lowest activation energies in virtue of cooperative H-bond effects.† We found that the structures determined in this way have the electrophile and nucleophile in a suitable configuration for the reaction to occur. This feature is one of the main attributes of bifunctional catalysts, *i.e.*, the placing of the reactants in an adequate disposition for the occurrence of the reaction.

We examined the topology of the electron density within the formalism of the Quantum Theory of Atoms In Molecules (QTAIM) to get further insights about the changes of the chemical bonding scenario associated to the reactions of interest. More precisely, we calculated QTAIM atomic charges together with electron delocalisation indices. All QTAIM calculations were carried out with the AIMAll program [9].

†The only exceptions to this statement are $C_2H_4O\cdots(H_2O)_5$ and (cis) 2,3-dimethyl oxirane$\cdots(H_2O)_5$ displayed in Figure S1 which present higher activation energies than the corresponding systems with four water molecules due to H-bond anticooperative effects.



(a) $C_2H_4O\cdots(H_2O)_4$ (b) $C_2H_4O\cdots(H_2O)_5$

(c) $(CH_3)_2C_2H_2O\cdots(H_2O)_5$ (d) $(CH_3)_2C_2H_2O\cdots(H_2O)_5$

Figure S1: Molecular clusters which lead to the hydrolysis of oxirane with $(H_2O)_4$ and $(H_2O)_5$.

Gibbs free energy profiles

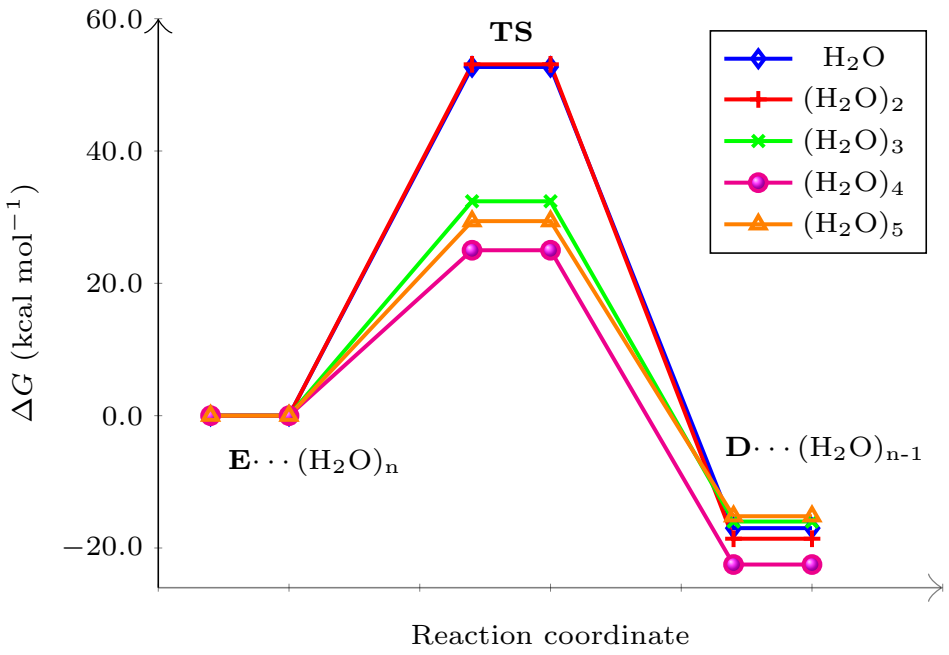


Figure S2: DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6−311++G(2d,2p) Gibbs free energy profiles at T = 373.15 K for the reaction of the molecular clusters comprised by one molecule of oxirane with n molecules of water (n = 1 − 5) to form ethylene glycol. The free energy values are referred to $G(C_2H_4O\cdots(H_2O)_n)$.

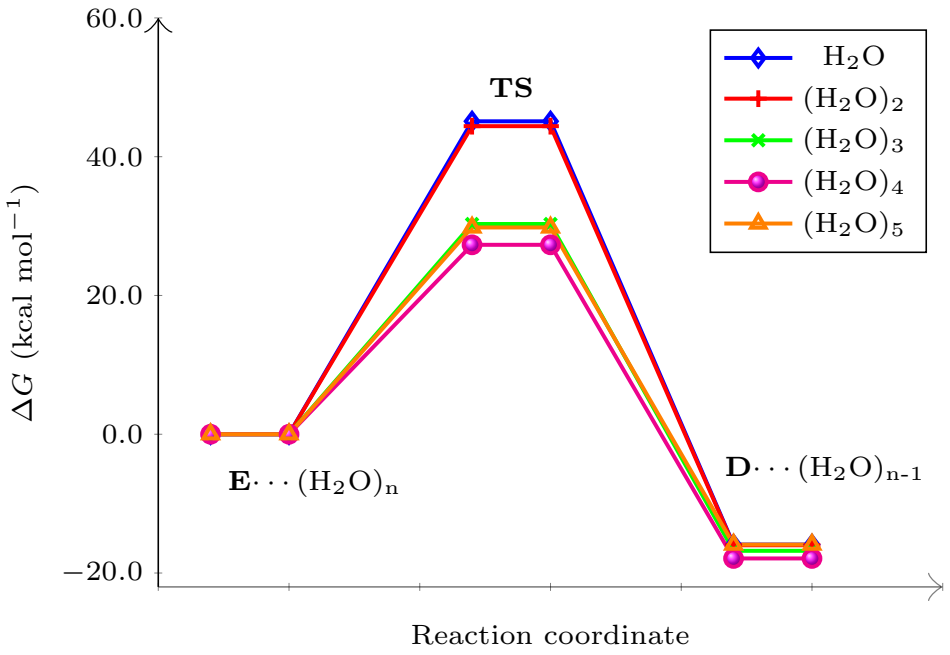


Figure S3: DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6−311++G(2d,2p) Gibbs free energy profiles at T = 333.15 K for the reaction of the molecular clusters comprised by one molecule of 2-methyl oxirane with n molecules of water (n = 1 – 5) to form 1,2-propanediol. The nucleophilic substitution occurs on the most substituted carbon atom. The free energy values are referred to G(2-methyl oxirane···$(H_2O)_n$).

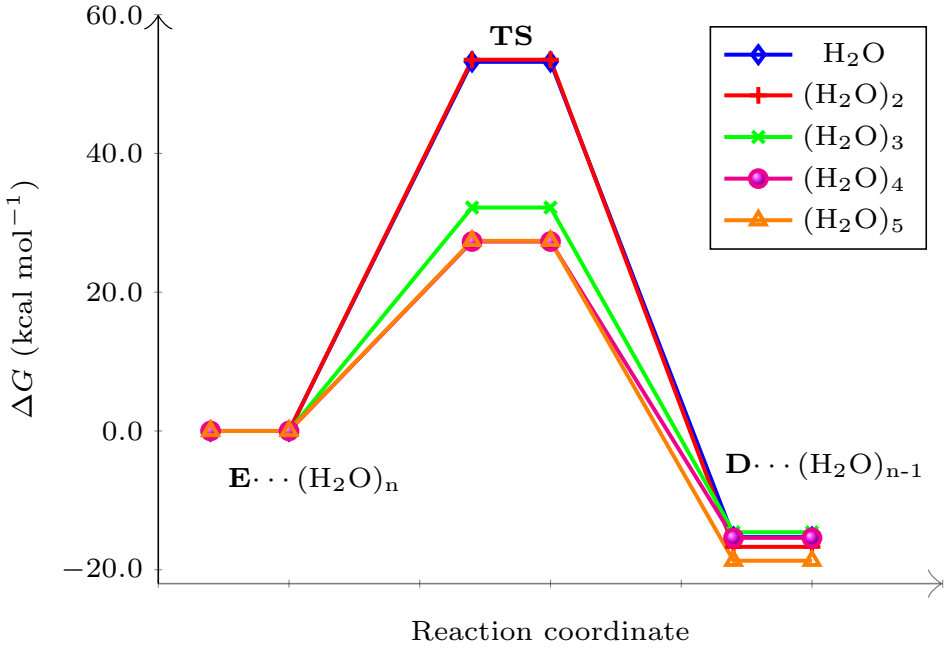


Figure S4: DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6−311++G(2d,2p) Gibbs free energy profiles at T = 333.15 K for the reaction of the molecular clusters comprised by one molecule of 2-methyl oxirane with n molecules of water (n = 1 – 5) to form 1,2-propanediol. The nucleophilic substitution occurs on the least substituted carbon atom The free energy values are referred to G(2-methyl oxirane···$(H_2O)_n$).

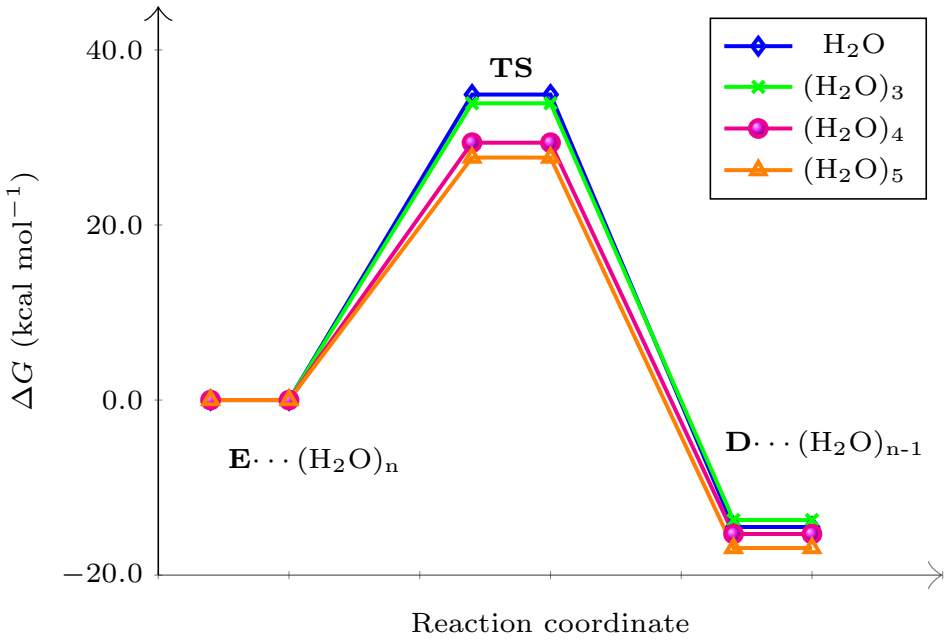


Figure S5: DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6−311++G(2d,2p) Gibbs free energy profiles at T = 333.15 K for the reaction of the molecular clusters comprised by one molecule of 2,2-dimethyl oxirane with n molecules of water (n = 1, 3−5) to form 2-methyl-1,2-propanediol. The nucleophilic substitution occurs on the most substituted carbon atom. The free energy values are referred to G(2,2-dimethyl oxirane···$(H_2O)_n$).

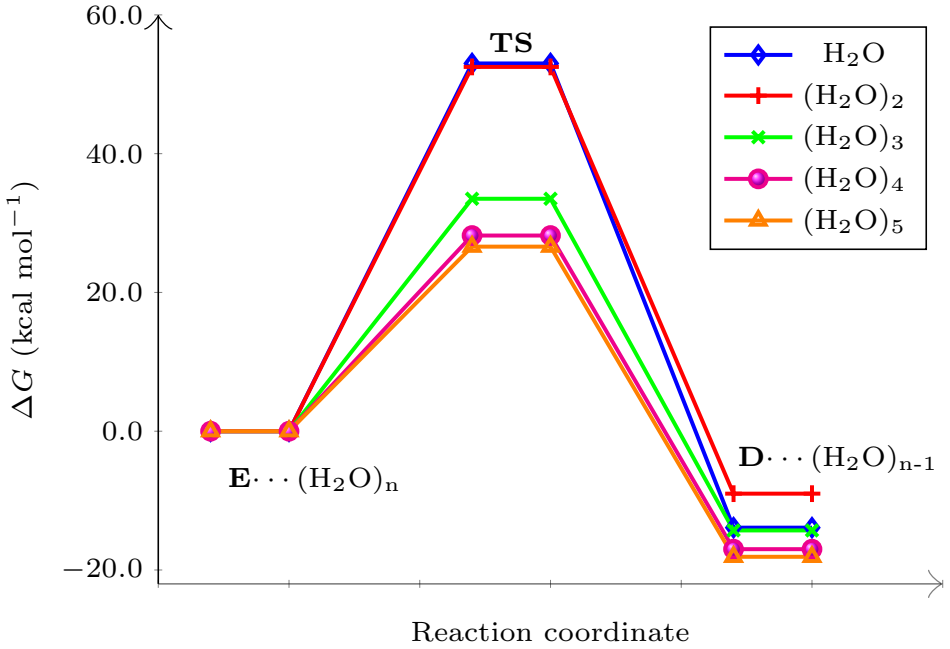


Figure S6: DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6−311++G(2d,2p) Gibbs free energy profiles at T = 333.15 K for the reaction of the molecular clusters comprised by one molecule of 2,2-dimethyl oxirane with n molecules of water (n = 1−5) to form 2-methyl-1,2-propanediol. The nucleophilic substitution occurs on the least substituted carbon atom. The free energy values are referred to G(2,2-dimethyl oxirane···$(H_2O)_n$).

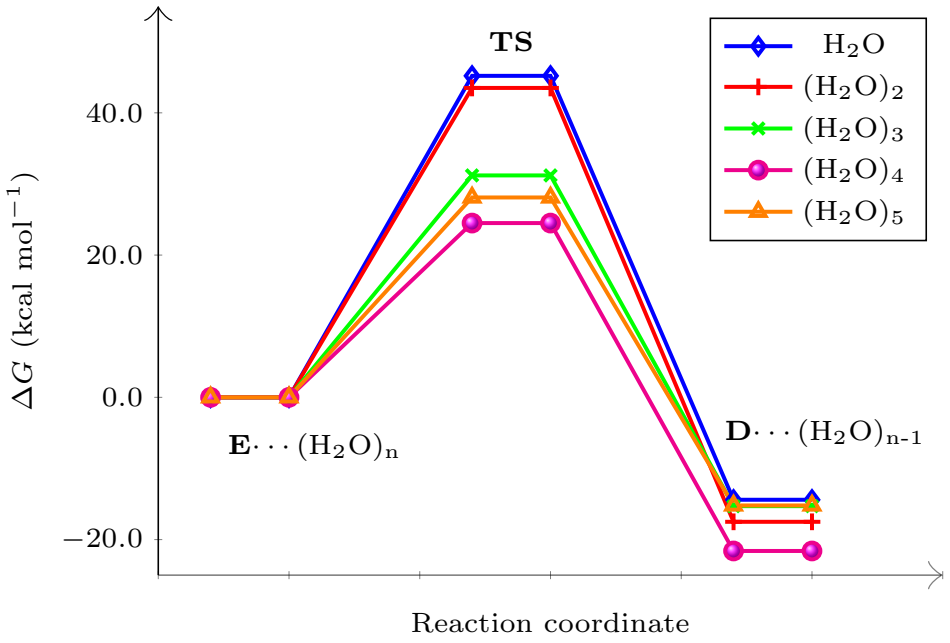


Figure S7: DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6–311++G(2d,2p) Gibbs free energy profiles at T = 333.15 K for the reaction of the molecular clusters comprised by one molecule of cis 2,3-dimethyl oxirane with n molecules of water (n = 1 – 5) to form 2,3-butanediol. The free energy values are referred to G(cis 2,3-dimethyl oxirane···$(H_2O)_n$).

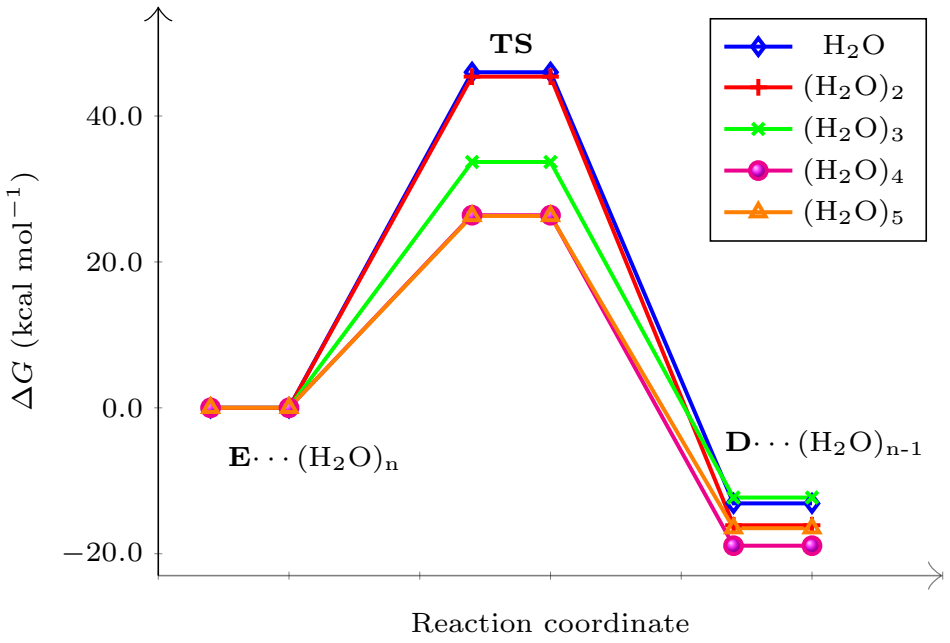


Figure S8: DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6–311++G(2d,2p) Gibbs free energy profiles at T = 333.15 K for the reaction of the molecular clusters comprised by one molecule of trans 2,3-dimethyl oxirane with n molecules of water (n = 1 – 5) to form 2,3-butanediol. The free energy values are referred to G(trans 2,3-dimethyl oxirane···$(H_2O)_n$).

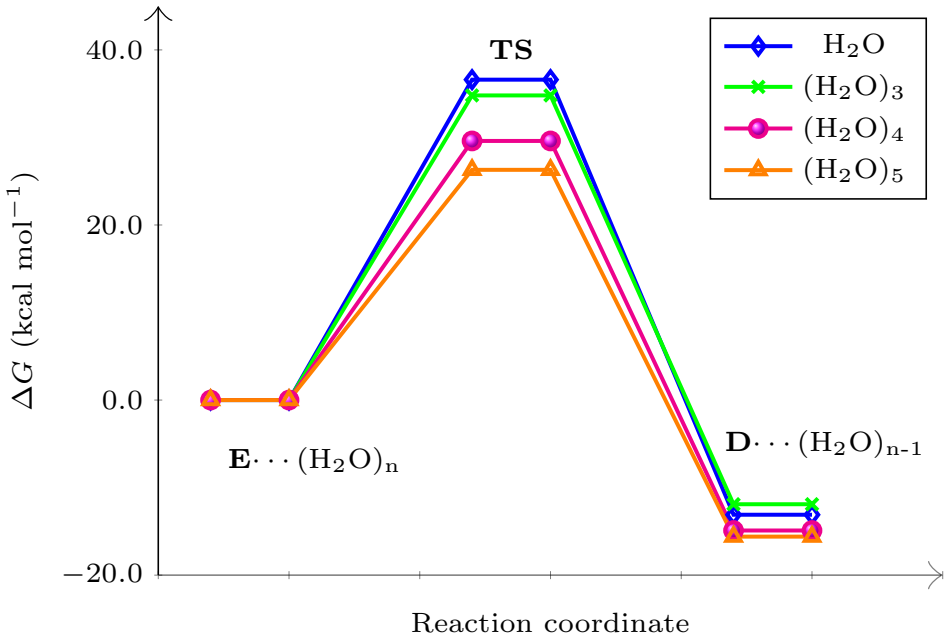


Figure S9: DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6–311++G(2d,2p) Gibbs free energy profiles at T = 333.15 K for the reaction of the molecular clusters comprised by one molecule of 2,3,3-trimethyl oxirane with n molecules of water (n = 1, 3 – 5) to form 2-methyl-2,3-butanediol. The nucleophilic substitution occurs on the most substituted carbon atom. The free energy values are referred to G(2,3,3-trimethyl oxirane···$(H_2O)_n$).

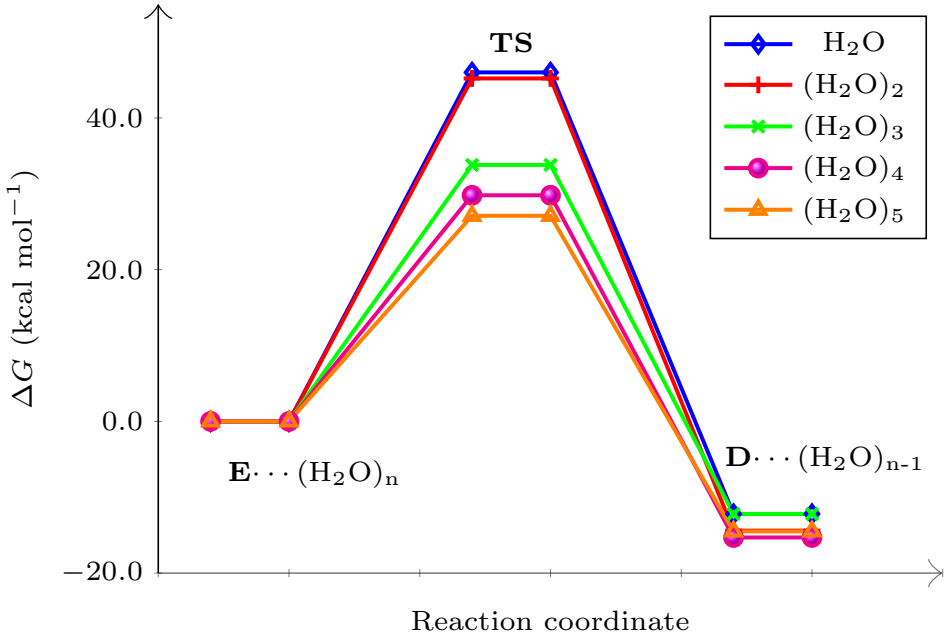


Figure S10: DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6–311++G(2d,2p) Gibbs free energy profiles at T = 333.15 K for the reaction of the molecular clusters comprised by one molecule of 2,3,3-trimethyl oxirane with n molecules of water (n = 1 – 5) to form 2-methyl-2,3-butanediol. The nucleophilic substitution occurs on the least substituted carbon atom. The free energy values are referred to G(2,3,3-trimethyl oxirane···$(H_2O)_n$).

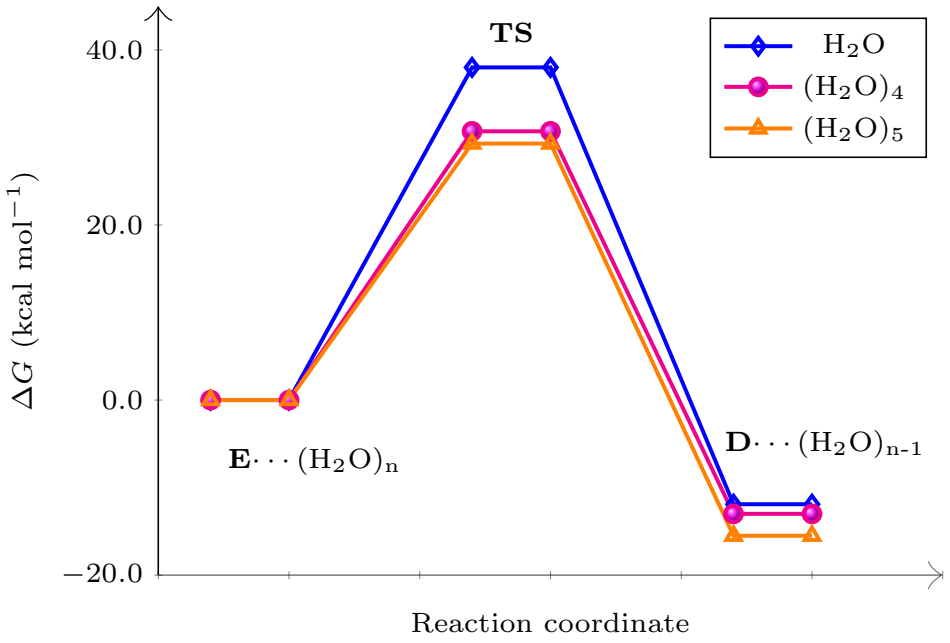


Figure S11: DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6−311++G(2d,2p) Gibbs free energy profiles at T = 333.15 K for the reaction of the molecular clusters comprised by one molecule of 2,3,3,3-tetramethyl oxirane with n molecules of water (n = 1, 4, 5) to form 2,3-dimethyl-2,3-butanediol. The free energy values are referred to G(2,3,3,3-tetramethyl oxirane···$(H_2O)_n$).

Table S1: Activation energies computed with the DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2d,2p) approximation for the hydrolyses of oxirane within its molecular cluster with n molecules of water (n = 1 – 5) at T = 373.15 K. The values are reported in kcal/mol.

System	ΔE_{act}	ΔG_{act}	ΔH_{act}	$-T\Delta S_{act}$
$C_2H_4O+H_2O$	52.26	52.74	49.96	2.77
$C_2H_4O+(H_2O)_2$	51.21	53.11	48.92	4.19
$C_2H_4O+(H_2O)_3$	27.87	32.39	27.38	5.02
$C_2H_4O+(H_2O)_4$	23.75	25.00	24.02	0.98
$C_2H_4O+(H_2O)_5$	27.83	29.43	26.23	3.20

Table S2: Activation energies computed with the DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2d,2p) approximation for the hydrolyses of 2-methyloxirane within its molecular cluster with n molecules of water (n = 1−5) at T = 333.15 K. The nucleophilic substitution occurs on the most substituted carbon atom. The values are reported in kcal/mol.

System	ΔE_{act}	ΔG_{act}	ΔH_{act}	$-T\Delta S_{act}$
$C_3H_6O+H_2O$	46.44	45.09	44.35	0.75
$C_3H_6O+(H_2O)_2$	45.59	44.39	42.47	1.92
$C_3H_6O+(H_2O)_3$	28.38	30.27	28.28	1.99
$C_3H_6O+(H_2O)_4$	26.34	27.27	25.55	1.72
$C_3H_6O+(H_2O)_5$	29.34	29.82	27.84	1.98

Table S3: Activation energies computed with the DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2d,2p) approximation for the hydrolyses of 2-methyloxirane within its molecular cluster with n molecules of water (n = 1−5) at T = 333.15 K. The nucleophilic substitution occurs on the least substituted carbon atom. The values are reported in kcal/mol.

System	ΔE_{act}	ΔG_{act}	ΔH_{act}	$-T\Delta S_{\mathrm{act}}$
$C_3H_6O+H_2O$	52.45	53.21	51.13	2.08
$C_3H_6O+(H_2O)_2$	51.10	53.48	49.80	3.68
$C_3H_6O+(H_2O)_3$	27.45	32.23	27.18	5.04
$C_3H_6O+(H_2O)_4$	24.86	27.33	23.48	3.85
$C_3H_6O+(H_2O)_5$	24.90	27.36	23.78	3.57

Table S4: Activation energies computed with the DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2d,2p) approximation for the hydrolyses of 2,2-dimethyloxirane within its molecular cluster with n molecules of water (n = 1, 3 – 5) at T = 333.15 K. The nucleophilic substitution occurs on the most substituted carbon atom. The values are reported in kcal/mol.

System	ΔE_{act}	ΔG_{act}	ΔH_{act}	$-T\Delta S_{\mathrm{act}}$
$C_4H_8O+H_2O$	35.78	34.87	32.88	1.99
$C_4H_8O+(H_2O)_3$	32.77	33.86	32.05	1.81
$C_4H_8O+(H_2O)_4$	27.33	29.43	24.98	4.45
$C_4H_8O+(H_2O)_5$	26.89	27.72	25.06	2.66

Table S5: Activation energies computed with the DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2d,2p) approximation for the hydrolyses of 2,2-dimethyloxirane within its molecular cluster with n molecules of water (n = 1 – 5) at T = 333.15 K. The nucleophilic substitution occurs on the least substituted carbon atom. The values are reported in kcal/mol.

System	ΔE_{act}	ΔG_{act}	ΔH_{act}	$-T\Delta S_{\mathrm{act}}$
$C_4H_8O+H_2O$	52.79	53.02	51.21	1.82
$C_4H_8O+(H_2O)_2$	51.42	52.49	50.06	2.42
$C_4H_8O+(H_2O)_3$	29.84	33.47	29.59	3.88
$C_4H_8O+(H_2O)_4$	24.91	28.20	23.71	4.49
$C_4H_8O+(H_2O)_5$	26.74	26.63	25.58	1.05

Table S6: Activation energies computed with the DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2d,2p) approximation for the hydrolyses of cis 2,3-dimethyloxirane within its molecular cluster with n molecules of water (n = 1−5) at T = 333.15 K. The values are reported in kcal/mol.

System	ΔE_{act}	ΔG_{act}	ΔH_{act}	$-T\Delta S_{\mathrm{act}}$
$C_4H_8O+H_2O$	45.65	45.19	43.65	1.54
$C_4H_8O+(H_2O)_2$	44.31	43.52	41.29	2.23
$C_4H_8O+(H_2O)_3$	27.67	31.16	27.60	3.56
$C_4H_8O+(H_2O)_4$	24.94	24.54	22.63	1.91
$C_4H_8O+(H_2O)_5$	28.34	28.12	26.77	1.35

Table S7: Activation energies computed with the DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2d,2p) approximation for the hydrolyses of trans 2,3-dimethyloxirane within its molecular cluster with n molecules of water (n = 1 – 5) at T = 333.15 K. The values are reported in kcal/mol.

System	ΔE_{act}	ΔG_{act}	ΔH_{act}	$-T\Delta S_{\mathrm{act}}$
$C_4H_8O+H_2O$	46.48	46.02	44.31	1.71
$C_4H_8O+(H_2O)_2$	46.21	45.42	42.98	2.43
$C_4H_8O+(H_2O)_3$	30.23	33.72	29.32	4.40
$C_4H_8O+(H_2O)_4$	26.76	26.37	25.41	0.96
$C_4H_8O+(H_2O)_5$	26.48	26.27	24.60	1.67

Table S8: Activation energies computed with the DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2d,2p) approximation for the hydrolyses of 2,2,3-trimethyloxirane within its molecular cluster with n molecules of water (n = 1, 3 – 5) at T = 333.15 K. The nucleophilic substitution occurs on the most substituted carbon atom. The values are reported in kcal/mol.

System	ΔE_{act}	ΔG_{act}	ΔH_{act}	$-T\Delta S_{\mathrm{act}}$
$C_5H_{10}O+H_2O$	36.52	36.59	33.84	2.75
$C_5H_{10}O+(H_2O)_3$	32.18	34.82	31.70	3.12
$C_5H_{10}O+(H_2O)_4$	27.19	29.60	25.58	4.02
$C_5H_{10}O+(H_2O)_5$	26.21	26.33	24.22	2.11

Table S9: Activation energies computed with the DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2d,2p) approximation for the hydrolyses of 2,2,3-trimethyloxirane within its molecular cluster with n molecules of water (n = 1 – 5) at T = 333.15 K. The nucleophilic substitution occurs on the least substituted carbon atom. The values are reported in kcal/mol.

System	ΔE_{act}	ΔG_{act}	ΔH_{act}	$-T\Delta S_{\mathrm{act}}$
$C_5H_{10}O+H_2O$	46.50	45.98	43.62	2.37
$C_5H_{10}O+(H_2O)_2$	45.96	45.25	43.05	2.20
$C_5H_{10}O+(H_2O)_3$	29.94	33.76	29.22	4.55
$C_5H_{10}O+(H_2O)_4$	26.33	29.83	25.00	4.84
$C_5H_{10}O+(H_2O)_5$	26.26	27.11	24.59	2.53

Table S10: Activation energies computed with the DLNPO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2d,2p) approximation for the hydrolyses of 2,2,3,3-tetramethyloxirane within its molecular cluster with n molecules of water (n = 1, 4, 5) at T = 333.15 K. The values are reported in kcal/mol.

System	ΔE_{act}	ΔG_{act}	ΔH_{act}	$-T\Delta S_{act}$
$C_6H_{12}O+H_2O$	37.60	37.98	34.62	3.36
$C_6H_{12}O+(H_2O)_4$	28.13	30.70	26.80	3.90
$C_6H_{12}O+(H_2O)_5$	25.78	29.31	23.74	5.57

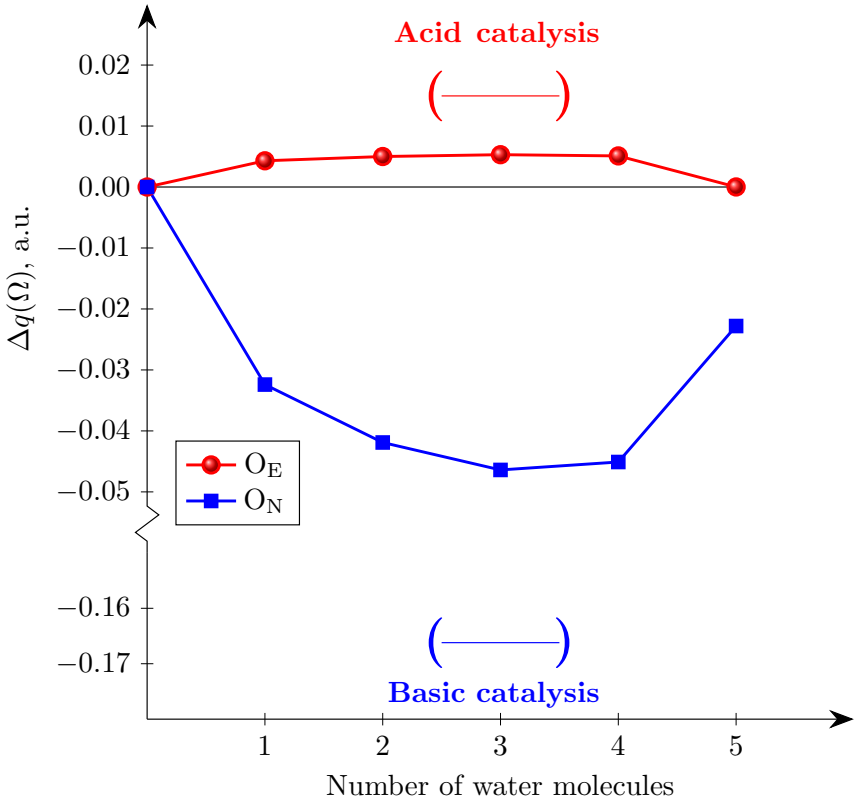


Figure S12: QTAIM charges of the nucleophilic atom (O_N) and the leaving oxygen (O_E) with respect to isolated H_2O and oxirane monomers respectively, within the molecular clusters $(CH_2)_2O\cdots(H_2O)_n$ (n = 1 – 5). The values corresponding to basic and acid catalysis with three water molecules are shown with blue and red horizontal lines respectively.

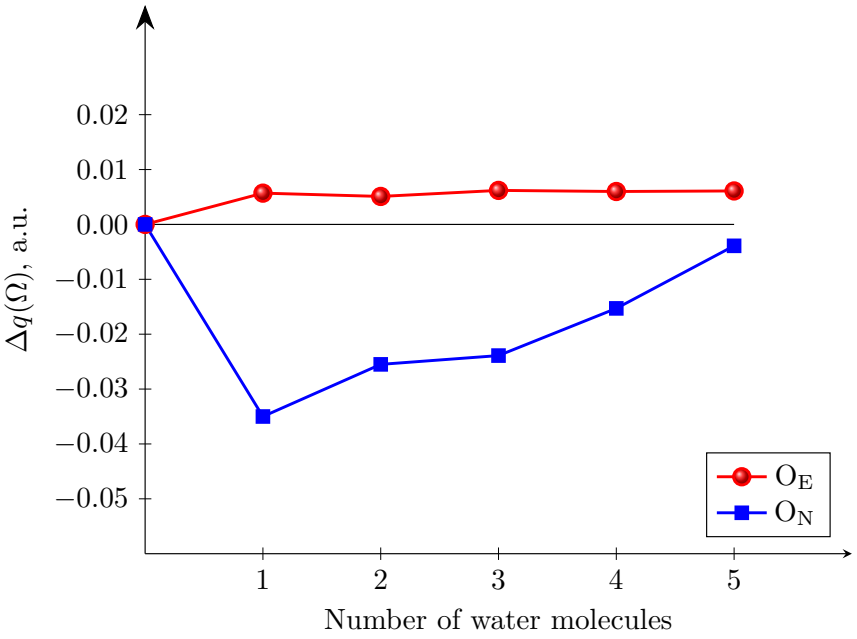


Figure S13: QTAIM charges of the nucleophilic atom (O_N) and the leaving oxygen (O_E) with respect to isolated H_2O and 2-methyloxirane monomers respectively, within the molecular clusters 2-methyloxirane···$(H_2O)_n$ (n = 1 – 5). The nucleophilic substitution occurs on the most substituted carbon atom.

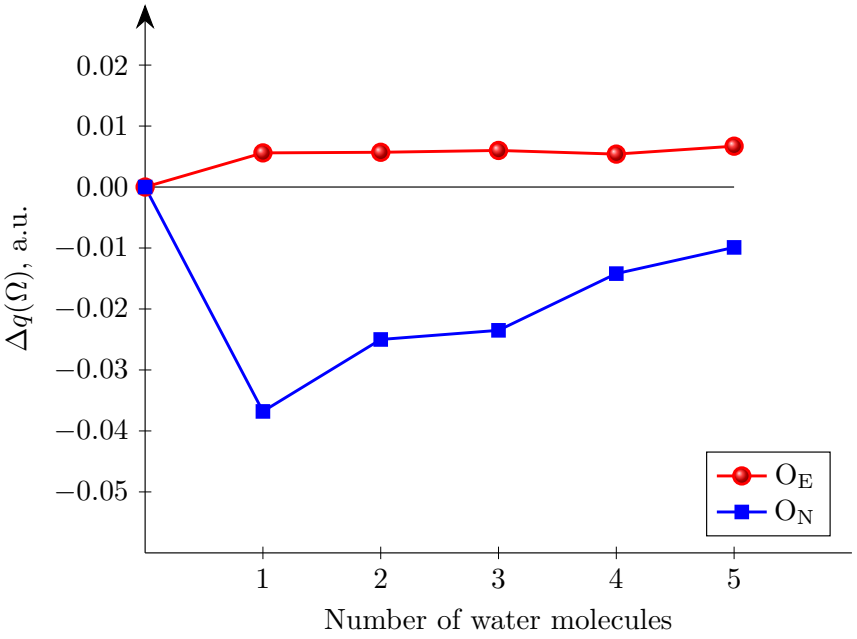


Figure S14: QTAIM charges of the nucleophilic atom (O_N) and the leaving oxygen (O_E) with respect to isolated H_2O and 2-methyloxirane monomers respectively, within the molecular clusters 2-methyloxirane···$(H_2O)_n$ (n = 1 – 5). The nucleophilic substitution occurs on the least substituted carbon atom.

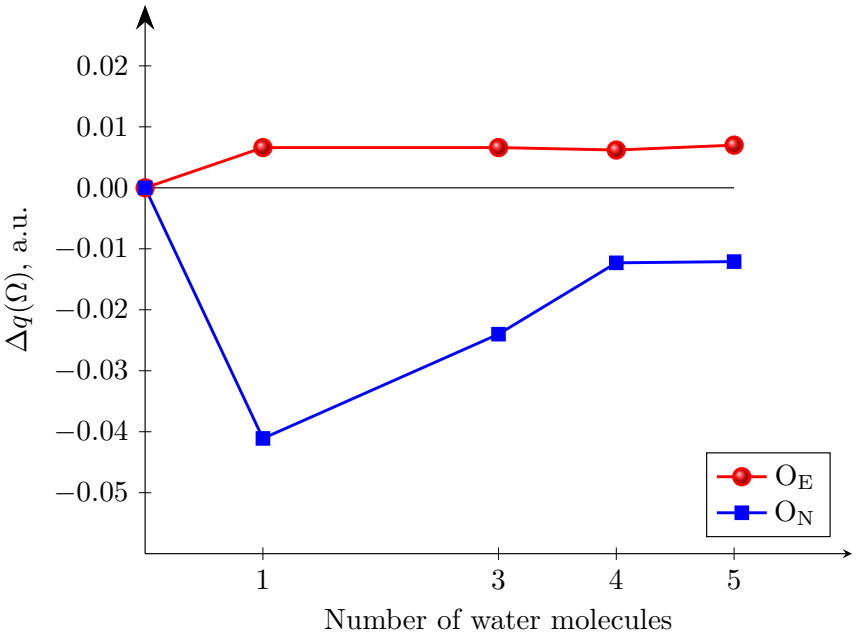


Figure S15: QTAIM charges of the nucleophilic atom (O_N) and the leaving oxygen (O_E) with respect to isolated H_2O and 2,2-dimethyloxirane monomers respectively, within the molecular clusters 2,2-dimethyloxirane···$(H_2O)_n$ (n = 1, 3 – 5). The nucleophilic substitution occurs on the most substituted carbon atom.

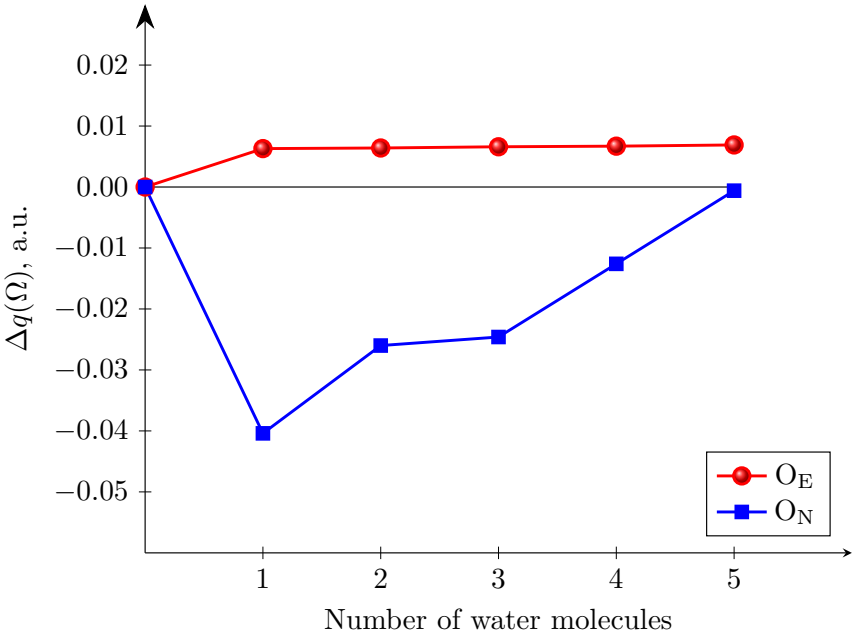


Figure S16: QTAIM charges of the nucleophilic atom (O_N) and the leaving oxygen (O_E) with respect to isolated H_2O and 2,2-dimethyloxirane monomers respectively, within the molecular clusters 2,2-dimethyloxirane···$(H_2O)_n$ (n = 1 – 5). The nucleophilic substitution occurs on the least substituted carbon atom.

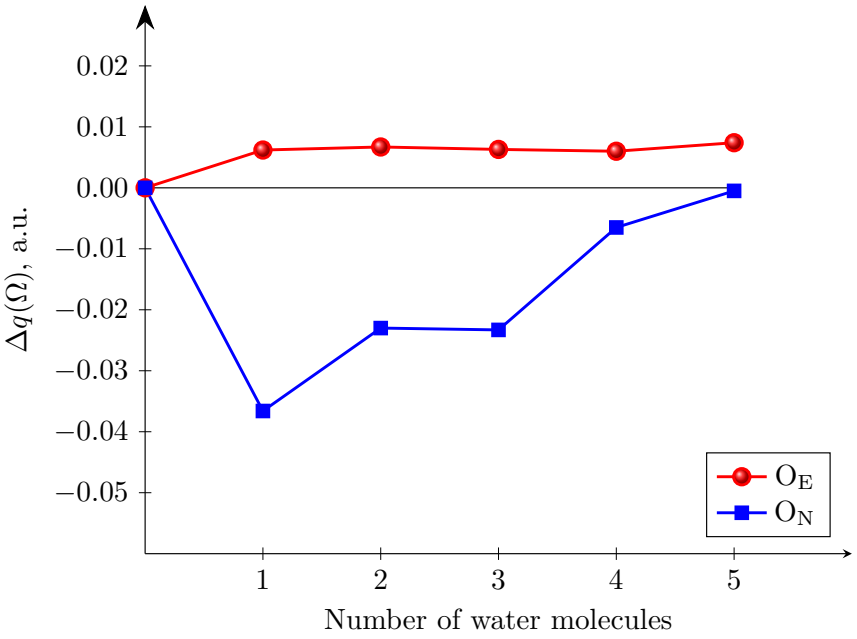


Figure S17: QTAIM charges of the nucleophilic atom (O_N) and the leaving oxygen (O_E) with respect to isolated H_2O and cis 2,3-dimethyloxirane monomers respectively, within the molecular clusters cis 2,3-dimethyloxirane···$(H_2O)_n$ (n = 1 – 5).

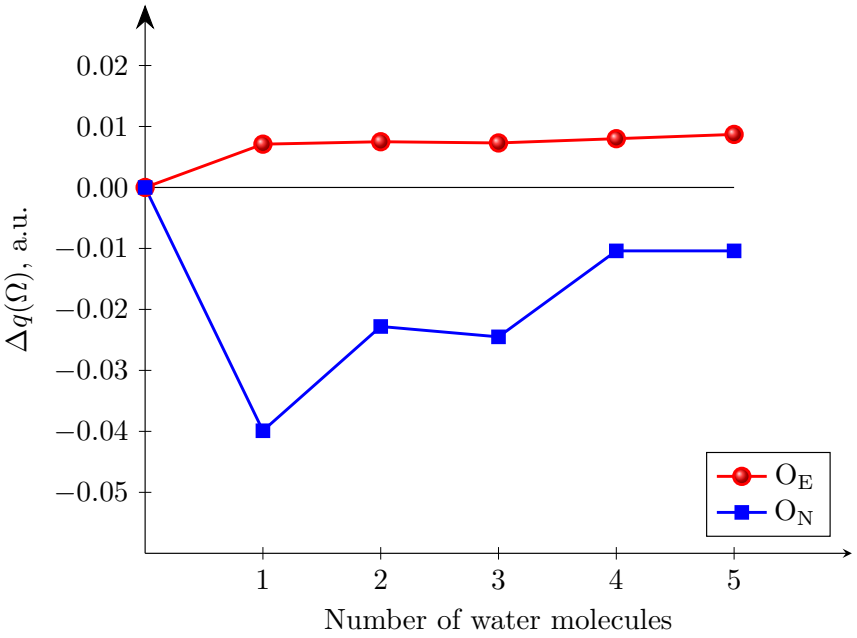


Figure S18: QTAIM charges of the nucleophilic atom (O_N) and the leaving oxygen (O_E) with respect to isolated H_2O and trans 2,3-dimethyloxirane monomers respectively, within the molecular clusters trans 2,3-dimethyloxirane···$(H_2O)_n$ (n = 1 – 5).

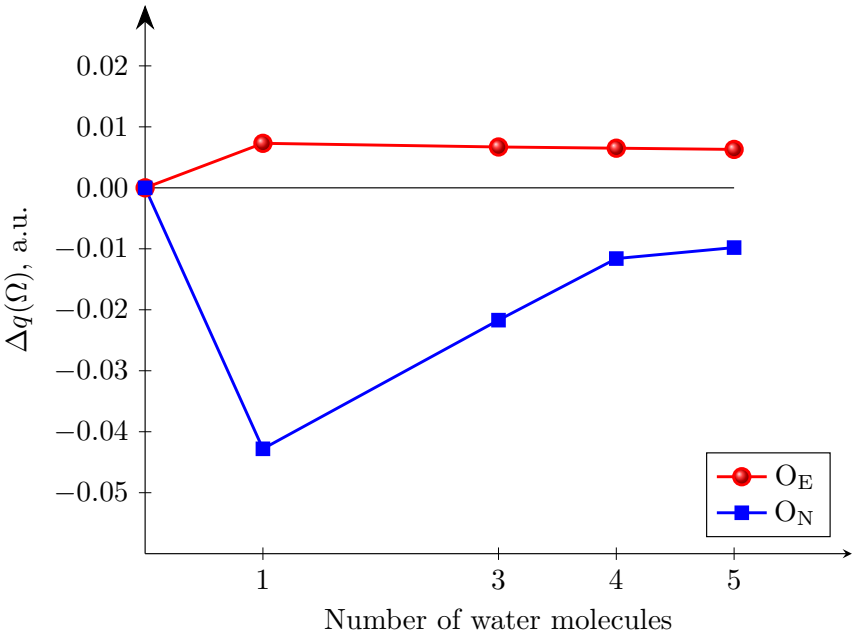


Figure S19: QTAIM charges of the nucleophilic atom (O_N) and the leaving oxygen (O_E) with respect to isolated H_2O and 2,2,3-trimethyloxirane monomers respectively, within the molecular clusters 2,2,3-trimethyloxirane···$(H_2O)_n$ (n = 1, 3 – 5). The nucleophilic substitution occurs on the most substituted carbon atom.

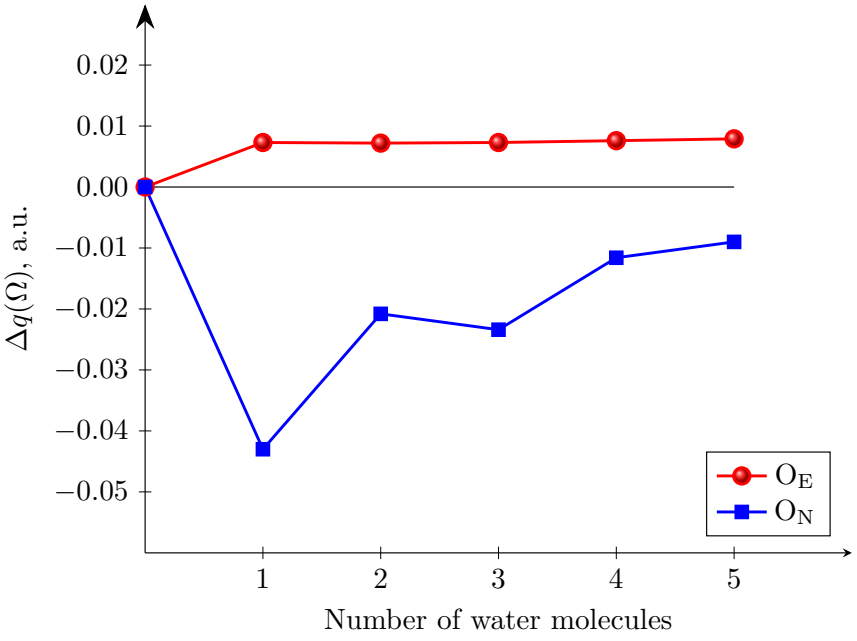


Figure S20: QTAIM charges of the nucleophilic atom (O_N) and the leaving oxygen (O_E) with respect to isolated H_2O and 2,2,3-trimethyloxirane monomers respectively, within the molecular clusters 2,2,3-trimethyloxirane···$(H_2O)_n$ (n = 1 – 5). The nucleophilic substitution occurs on the least substituted carbon atom.

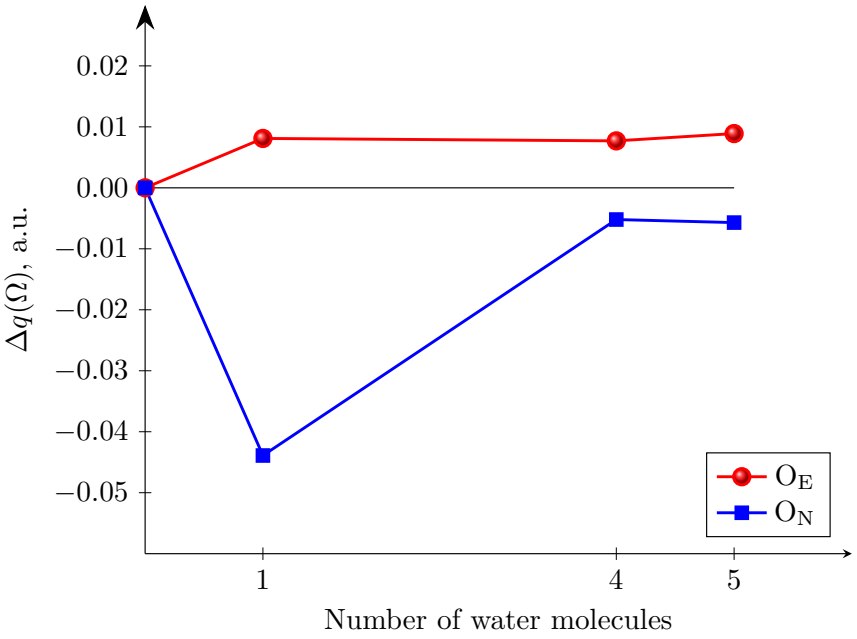


Figure S21: QTAIM charges of the nucleophilic atom (O_N) and the leaving oxygen (O_E) with respect to isolated H_2O and 2,2,3,3-tetramethyloxirane monomers respectively, within the molecular clusters 2,2,3,3-tetramethyloxirane···$(H_2O)_n$ (n = 1, 4, 5).

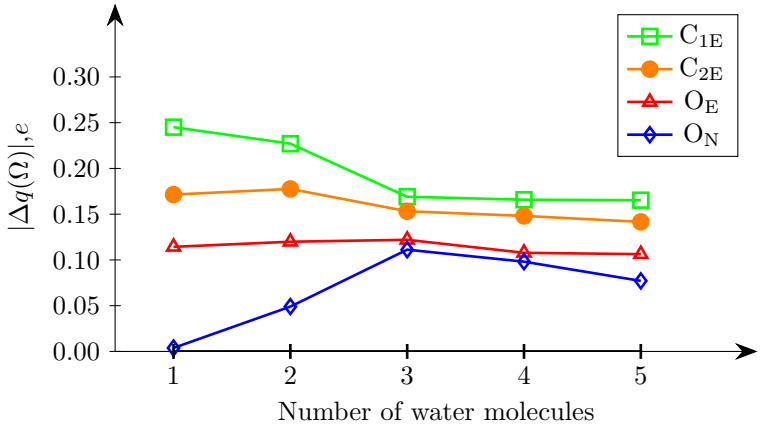


Figure S22: Values of $|\Delta q(\Omega)|$ of the atoms directly involved in the epoxide ring rupture for the investigated oxirane hydrolyses reactions. The labels C_{1E}, C_{2E}, O_E and O_N are defined in Figure 4 (a) in the body of the paper.

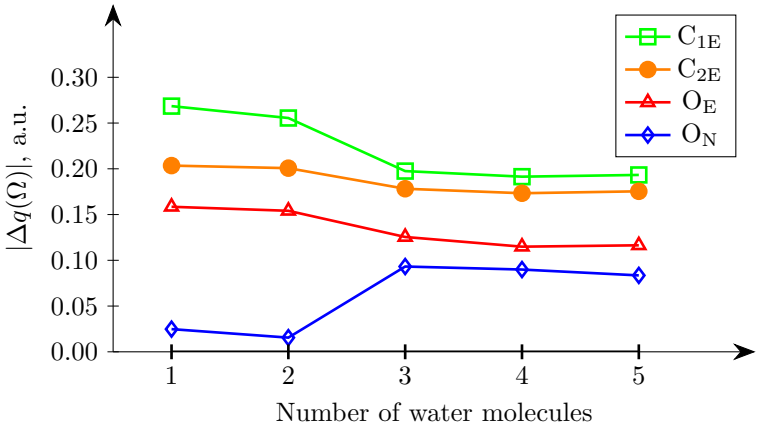


Figure S23: Values of $|\Delta q(\Omega)|$ of the atoms directly involved in the epoxide ring rupture for the investigated 2-methyloxirane hydrolyses reactions. The labels C_{1E}, C_{2E}, O_E and O_N are defined in Figure 4 (a) in the body of the paper. The nucleophilic substitution occurs on the most substituted carbon atom.

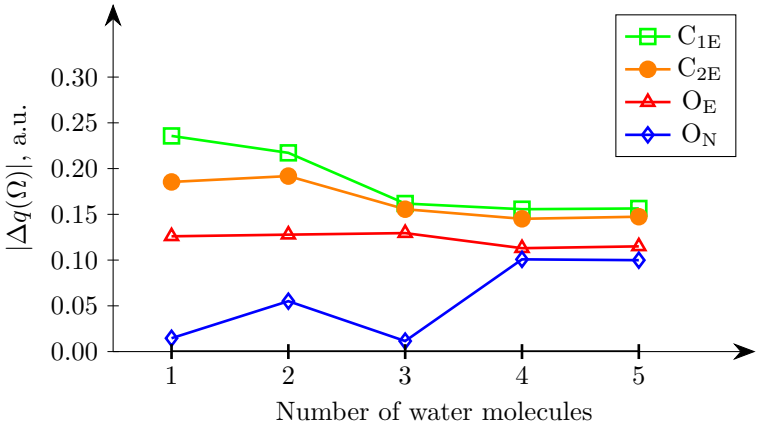


Figure S24: Values of $|\Delta q(\Omega)|$ of the atoms directly involved in the epoxide ring rupture for the investigated 2-methyloxirane hydrolyses reactions. The labels C_{1E}, C_{2E}, O_E and O_N are defined in Figure 4 (a) in the body of the paper. The nucleophilic substitution occurs on the least substituted carbon atom.

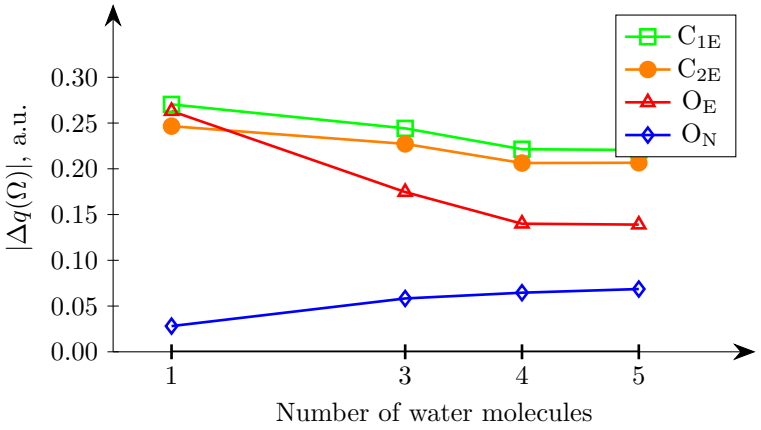


Figure S25: Values of $|\Delta q(\Omega)|$ of the atoms directly involved in the epoxide ring rupture for the investigated 2,2-dimethyloxirane hydrolyses reactions. The labels C_{1E}, C_{2E}, O_E and O_N are defined in Figure 4 (a) in the body of the paper. The nucleophilic substitution occurs on the most substituted carbon atom.

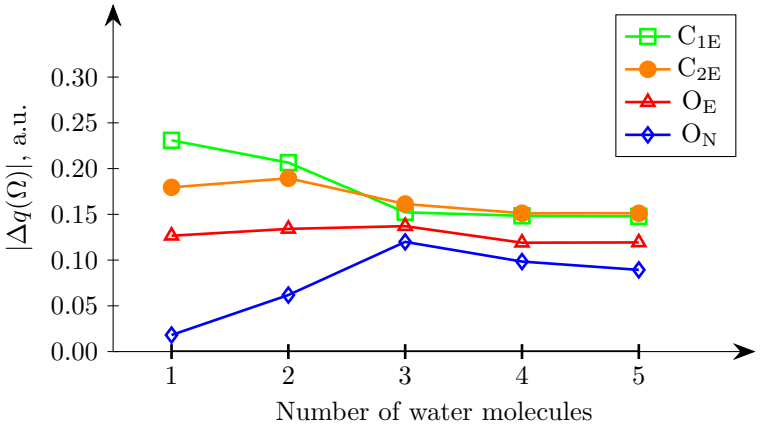


Figure S26: Values of $|\Delta q(\Omega)|$ of the atoms directly involved in the epoxide ring rupture for the investigated 2,2-dimethyloxirane hydrolyses reactions. The labels C_{1E}, C_{2E}, O_E and O_N are defined in Figure 4 (a) in the body of the paper. The nucleophilic substitution occurs on the most substituted carbon atom.

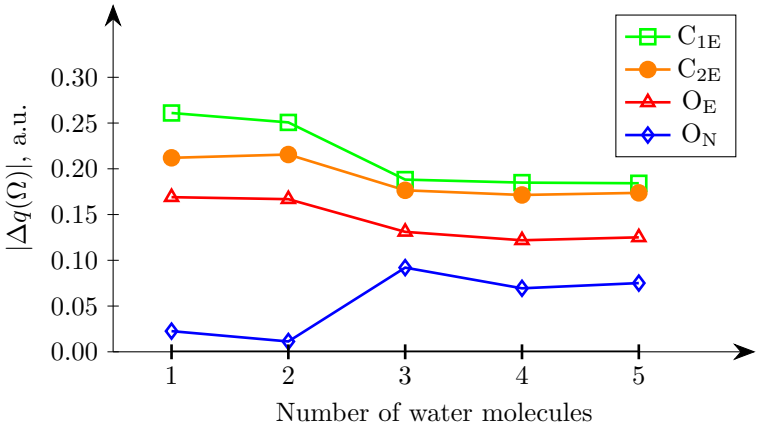


Figure S27: Values of $|\Delta q(\Omega)|$ of the atoms directly involved in the epoxide ring rupture for the investigated cis 2,3-dimethyloxirane hydrolyses reactions. The labels C_{1E}, C_{2E}, O_E and O_N are defined in Figure 4 (a) in the body of the paper.

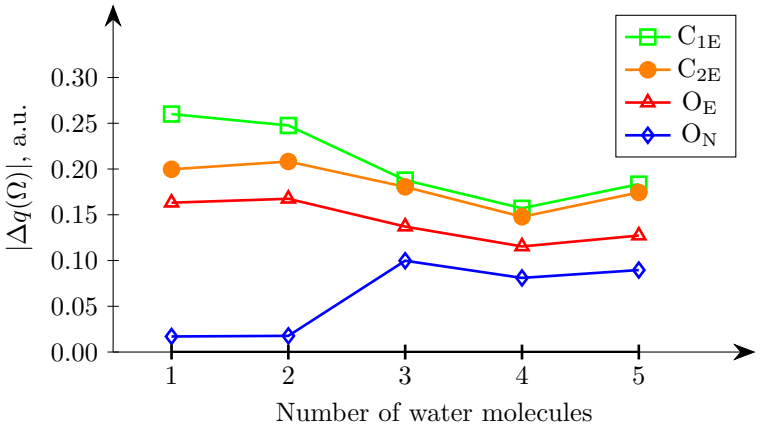


Figure S28: Values of $|\Delta q(\Omega)|$ of the atoms directly involved in the epoxide ring rupture for the investigated trans 2,3-dimethyloxirane hydrolyses reactions. The labels C_{1E}, C_{2E}, O_E and O_N are defined in Figure 4 (a) in the body of the paper.

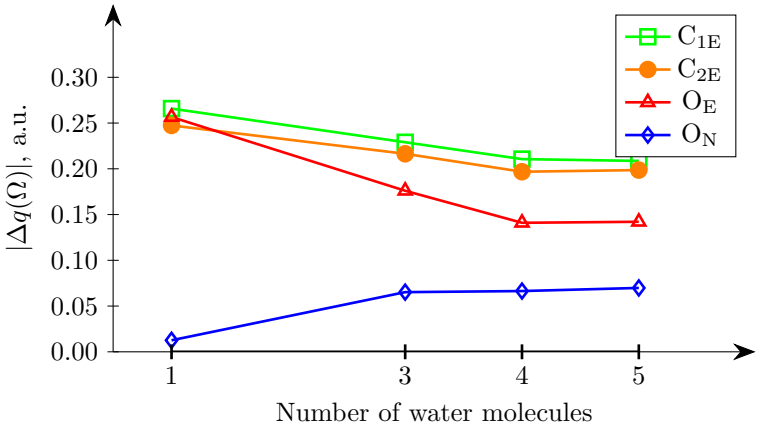


Figure S29: Values of $|\Delta q(\Omega)|$ of the atoms directly involved in the epoxide ring rupture for the investigated 2,2,3-trimethyloxirane hydrolyses reactions. The labels C_{1E}, C_{2E}, O_E and O_N are defined in Figure 4 (a) in the body of the paper. The nucleophilic substitution occurs on the most substituted carbon atom.

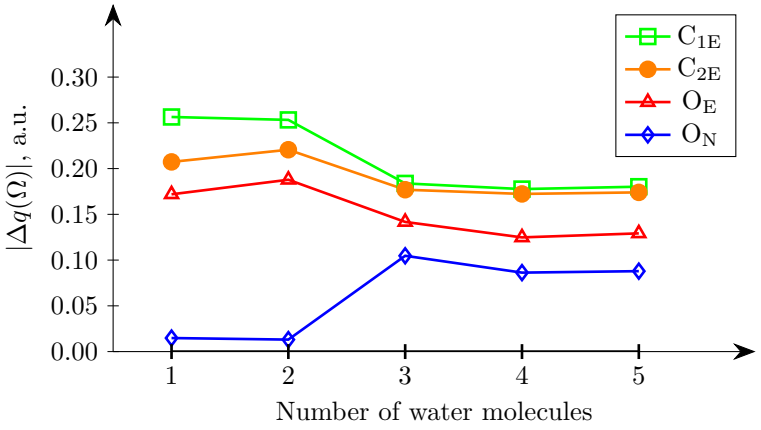


Figure S30: Values of $|\Delta q(\Omega)|$ of the atoms directly involved in the epoxide ring rupture for the investigated 2,2,3-trimethyloxirane hydrolyses reactions. The labels C_{1E}, C_{2E}, O_E and O_N are defined in Figure 4 (a) in the body of the paper. The nucleophilic substitution occurs on the least substituted carbon atom.

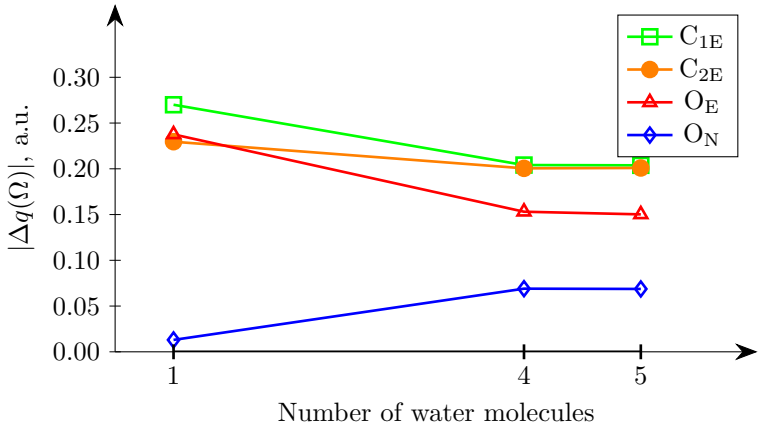


Figure S31: Values of $|\Delta q(\Omega)|$ of the atoms directly involved in the epoxide ring rupture for the investigated 2,2,3,3-tetramethyloxirane hydrolyses reactions. The labels C_{1E}, C_{2E}, O_E and O_N are defined in Figure 4 (a) in the body of the paper.

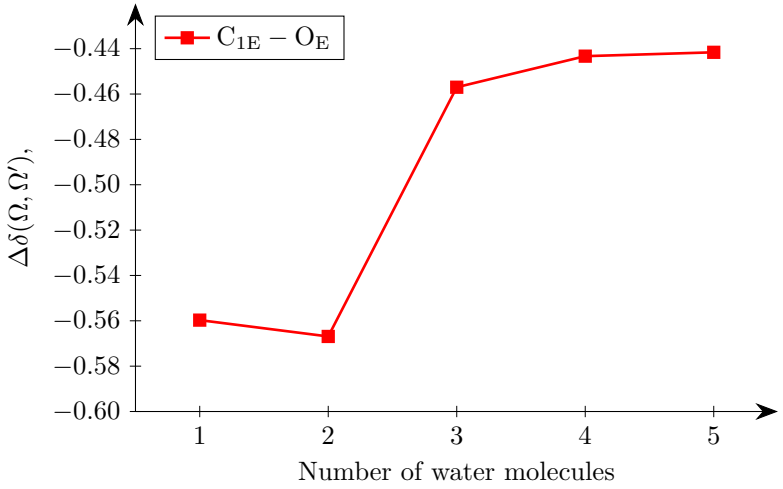


Figure S32: Values of $\Delta\delta(C_{1E},O_E)$ throughout the rate-limiting step of the hydrolyses of oxirane in its molecular clusters with n molecules of water (n = 1 – 5). The labels C_{1E} and O_E are defined in Figure 4 (a) in the body of the manuscript.

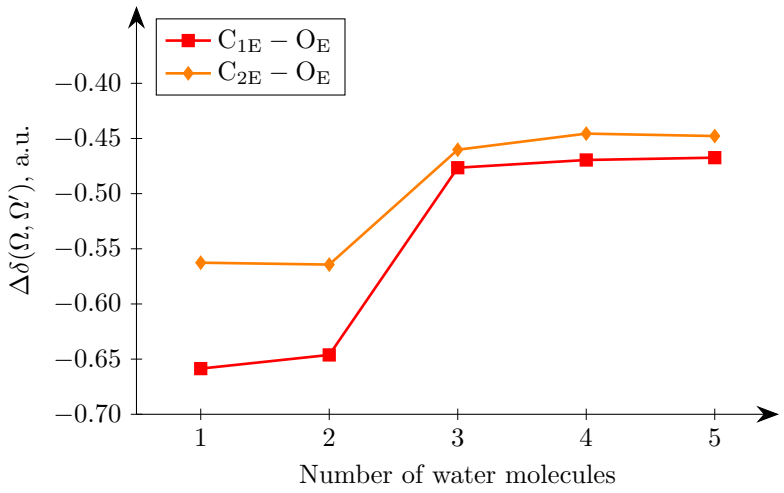


Figure S33: Values of $\Delta\delta(C_{1E},O_E)$ and $\Delta\delta(C_{2E},O_E)$ throughout the rate-limiting step of the hydrolyses of 2-methyloxirane in its molecular clusters with n molecules of water (n = 1 – 5). The labels C_{1E}, C_{2E} and O_E are defined in Figure 4 (a) in the body of the manuscript.

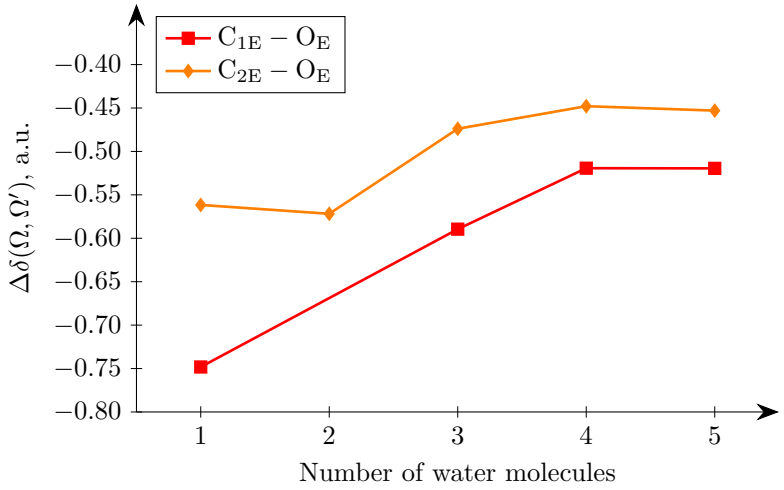


Figure S34: Values of $\Delta\delta(C_{1E},O_E)$ and $\Delta\delta(C_{2E},O_E)$ throughout the rate-limiting step of the hydrolyses of 2,2-dimethyloxirane in its molecular clusters with n molecules of water (n = 1–5). The labels C_{1E}, C_{2E} and O_E are defined in Figure 4 (a) in the body of the manuscript.

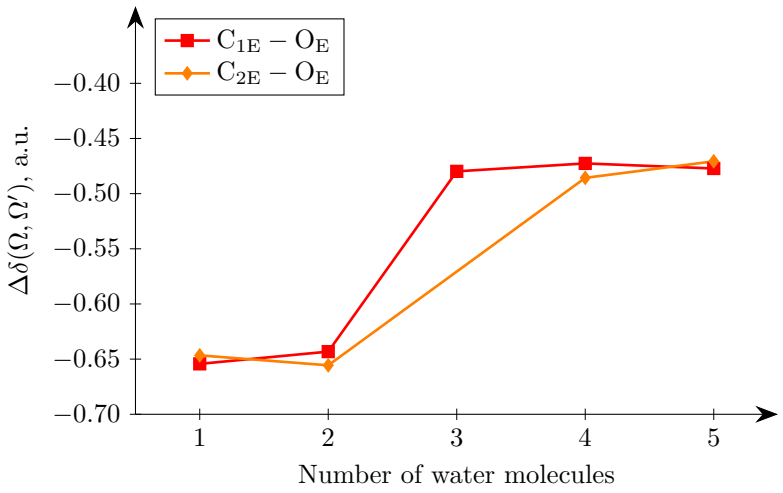


Figure S35: Values of $\Delta\delta(C_{1E},O_E)$ and $\Delta\delta(C_{2E},O_E)$ throughout the rate-limiting step of the hydrolyses of cis 2,3-dimethyloxirane in its molecular clusters with n molecules of water (n = 1 – 5). The labels C_{1E}, C_{2E} and O_E are defined in Figure 4 (a) in the body of the manuscript.

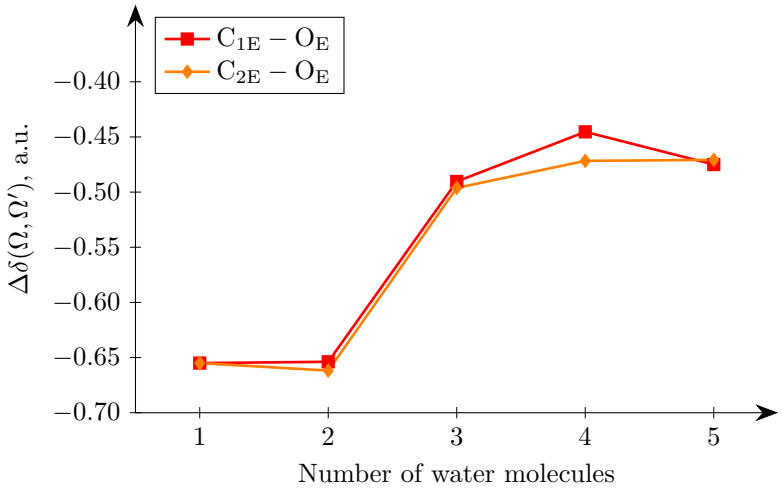


Figure S36: Values of $\Delta\delta(C_{1E},O_E)$ and $\Delta\delta(C_{2E},O_E)$ throughout the rate-limiting step of the hydrolyses of trans 2,3-dimethyloxirane in its molecular clusters with n molecules of water (n = 1 – 5). The labels C_{1E}, C_{2E} and O_E are defined in Figure 4 (a) in the body of the manuscript.

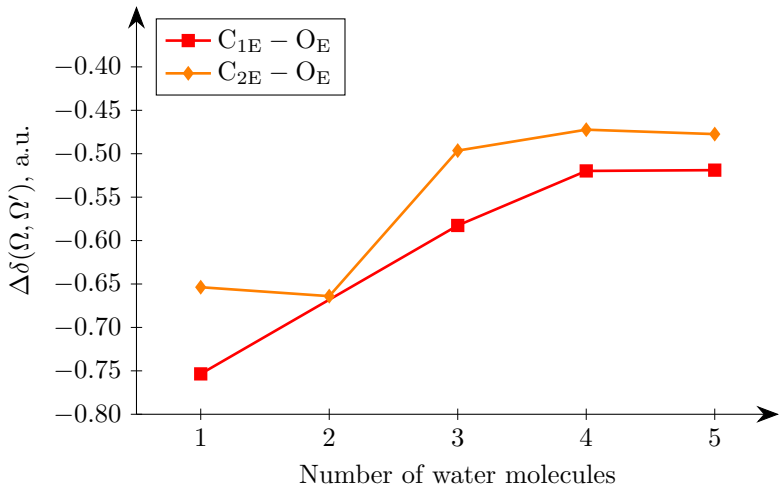


Figure S37: Values of $\Delta\delta(C_{1E},O_E)$ and $\Delta\delta(C_{2E},O_E)$ throughout the rate-limiting step of the hydrolyses of 2,2,3-trimethyloxirane in its molecular clusters with n molecules of water (n = 1 – 5). The labels C_{1E}, C_{2E} and O_E are defined in Figure 4 (a) in the body of the manuscript.

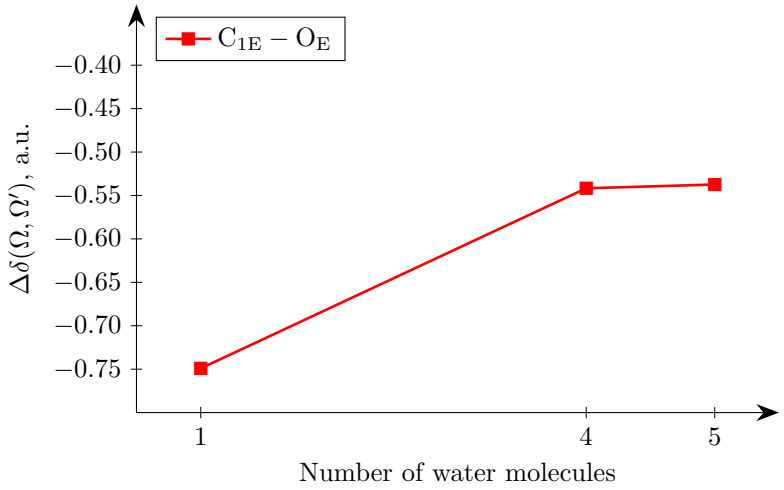


Figure S38: Values of $\Delta\delta(C_{1E},O_E)$ throughout the rate-limiting step of the hydrolyses of 2,2,3,3-tetramethyloxirane in its molecular clusters with n molecules of water (n = 1 – 5). The labels C_{1E}, C_{2E} and O_E are defined in Figure 4 (a) in the body of the manuscript.

DFT electronic energies and xyz coordinates (Å) of all systems addressed in this investigation.

Hydrolysis of C_2H_4O *at 373 K.*

$C_2H_4O\cdots H_2O$

```
E(RM062X) = -230.219688540
C       1.053583      0.747248      0.271450
H       0.327568      1.290870      0.861822
H       1.954271      1.277941     -0.003485
C       1.072199     -0.712320      0.338144
```

H	1.986838	-1.242007	0.111521
O	-2.228909	-0.021325	0.012021
H	-2.097513	0.201852	0.938354
O	0.484901	-0.039757	-0.784354
H	-1.333799	-0.031508	-0.363798
H	0.360011	-1.218065	0.976687

$C_2H_4O\cdots(H_2O)_2$

E(RM062X) = -306.662460352

C	-2.028649	0.156466	-0.267789
H	-1.865118	1.055021	-0.848142
H	-3.049636	-0.068397	0.006623
C	-1.051589	-0.927290	-0.349369
H	-0.186551	-0.805312	-0.988900
H	-1.361574	-1.940198	-0.134103
O	-1.074897	-0.047893	0.784501
H	1.819971	-1.553064	0.099081
O	2.503212	-0.883322	0.002168
H	2.018535	-0.041033	-0.033869
O	1.069648	1.572796	-0.016732
H	0.298200	1.132499	0.379752
H	0.823899	1.712784	-0.936982

$C_2H_4O\cdots(H_2O)_3$

E(RM062X) = -383.107330626

O	-2.729996	-0.549014	-0.076439
H	-2.256406	-1.343972	0.184559
H	-2.085757	0.175203	0.016918
O	-1.130930	1.755099	0.163030
H	-1.445596	2.305775	-0.560723
H	-0.164667	1.700155	0.037457
O	1.673389	-1.106792	-0.018485
O	1.654590	1.683404	-0.158379
H	1.873575	0.740310	-0.069520
H	2.011570	2.101008	0.631710
C	0.473425	-1.231080	0.758628
C	0.420039	-1.251305	-0.702392
H	0.094502	-0.362463	-1.227651
H	0.297896	-2.194902	-1.215658
H	0.186653	-0.328145	1.282635
H	0.391025	-2.160243	1.305037

$C_2H_4O\cdots(H_2O)_4$

E(RM062X) = -459.551229914

O	-3.014726	-0.607111	-0.565722
H	-2.611944	-1.420882	-0.249476
H	-2.542811	0.104229	-0.095224
O	-1.782790	1.534134	0.759501
H	-1.584269	1.195343	1.638060

H	-0.912369	1.688167	0.343568
O	0.604700	2.113436	-0.552832
H	0.373951	1.919473	-1.467089
H	1.358559	1.525090	-0.356520
O	1.219602	-1.799672	0.195889
O	2.827067	0.480037	-0.052761
H	2.444196	-0.402642	0.088296
H	3.181620	0.739223	0.803594
C	0.105533	-1.117696	0.792019
C	0.166194	-1.320311	-0.653732
H	0.446860	-0.491100	-1.290738
H	-0.428874	-2.102404	-1.105344
H	0.351078	-0.144279	1.197374
H	-0.537179	-1.748765	1.391175

$C_2H_4O\cdots(H_2O)_5$

E(RM062X) = -535.997091960

O	1.194473	-2.379477	0.016499
H	1.958350	-2.834366	0.385566
H	0.926353	-1.749452	0.705686
O	0.947437	-0.099131	1.775044
H	0.197690	0.486951	1.578270
H	1.632187	0.165286	1.143000
O	2.577395	0.126639	-0.657446
H	2.100635	-0.714191	-0.716910
H	1.925043	0.818701	-0.867012
O	0.772262	2.269572	-0.972255
H	1.301964	3.033144	-0.721441
H	0.126338	2.160755	-0.251667
O	-2.342412	-0.136323	-0.630271
O	-1.118653	1.695563	1.024389
H	-1.781687	1.209523	0.503538
H	-1.602222	2.323835	1.569431
C	-1.076837	-0.694925	-1.016730
C	-1.874866	-1.322260	0.032213
H	-1.592030	-1.171989	1.066429
H	-2.444367	-2.212711	-0.194307
H	-0.218117	-0.098093	-0.734387
H	-1.063924	-1.129037	-2.006767

$[C_2H_4O\cdots H_2O]^{\ddagger}$

E(RM062X) = -230.132927339

C	0.275055	1.055187	-0.193090
H	-0.264111	1.722871	0.462177
H	0.103154	1.139452	-1.257473
C	1.251457	0.071558	0.253667
H	2.217928	0.232775	-0.239473
O	-1.737333	-0.100145	0.216297
H	-2.184983	-0.008270	-0.631267

O	0.553204	-1.051668	-0.225871
H	-0.953663	-0.710844	0.043168
H	1.395634	0.078059	1.336004

$[C_2H_4O\cdots(H_2O)_2]^{\ddagger}$

E(RM062X) = -306.578740164

C	1.330468	-0.732135	-0.273634
H	0.938711	-1.197769	-1.182474
H	2.346143	-1.109633	-0.094521
C	1.333829	0.720514	-0.348642
H	1.039296	1.283961	-1.220345
H	1.722760	1.264795	0.500272
O	0.471480	-0.840791	0.831229
H	-0.723113	1.702571	1.039835
O	-0.786656	1.670619	0.078871
H	-1.311530	0.867457	-0.101073
O	-1.851161	-0.901626	-0.200660
H	-0.924082	-0.957272	0.221284
H	-1.743272	-1.210000	-1.104846

$[C_2H_4O\cdots(H_2O)_3]^{\ddagger}$

E(RM062X) = -383.058521340

O	-2.083825	-0.655831	-0.252217
H	-2.371022	-1.134884	0.535564
H	-1.936571	0.276175	0.028788
O	-1.119754	1.830780	0.330114
H	-1.459069	2.501335	-0.271354
H	-0.173551	1.739872	0.104748
O	1.624951	-1.185850	-0.049750
O	1.641805	1.465740	-0.332396
H	1.778438	0.484227	-0.251841
H	2.125501	1.852766	0.403398
C	0.466904	-1.100057	0.750153
C	-0.234022	-1.065697	-0.526759
H	-0.131386	-0.182968	-1.135434
H	-0.399288	-2.003586	-1.032844
H	0.394534	-0.193609	1.354702
H	0.269697	-1.983518	1.357906

$[C_2H_4O\cdots(H_2O)_4]^{\ddagger}$

E(RM062X) = -459.505984281

O	-2.006398	-0.934990	-0.774348
H	-2.436978	-1.689499	-0.354007
H	-2.140449	-0.164751	-0.161005
O	-2.090696	1.194636	0.805585
H	-1.868168	0.867366	1.683246
H	-1.254490	1.563656	0.448691
O	0.135021	2.201597	-0.436274
H	-0.113229	2.089571	-1.359348

H	0.970358	1.693918	-0.333419
O	1.563102	-1.505065	0.267398
O	2.487878	0.838718	-0.156990
H	2.179316	-0.110295	0.027964
H	2.880902	1.150438	0.663398
C	0.291595	-1.212809	0.805021
C	-0.118926	-1.266908	-0.591647
H	0.130548	-0.422702	-1.215505
H	-0.199228	-2.237754	-1.051802
H	0.220723	-0.230952	1.277741
H	-0.116575	-1.989864	1.450831

$[C_2H_4O\cdots(H_2O)_5]^{\ddagger}$

E(RM062X) = -535.948229227

O	1.959034	-1.791357	-0.535158
H	2.113514	-2.249312	0.300302
H	0.997068	-1.915425	-0.744049
O	-0.631658	-1.835497	-1.132312
H	-0.745902	-0.947860	-1.492440
H	-1.094895	-1.807165	-0.273098
O	-2.022556	-1.475076	1.281108
H	-1.356044	-1.315015	1.956853
H	-2.200141	-0.599033	0.886002
O	-2.514187	0.793904	-0.234954
H	-2.724612	0.343727	-1.059476
H	-1.735693	1.355247	-0.442388
O	1.471483	1.692909	0.784018
O	-0.385322	2.412035	-0.837914
H	0.365650	2.211784	-0.190127
H	-0.676244	3.305311	-0.632844
C	1.044787	0.363674	0.991081
C	1.966364	0.081609	-0.100435
H	1.651635	0.344939	-1.097758
H	3.020903	0.086235	0.118642
H	-0.009903	0.194311	0.767301
H	1.313412	-0.054790	1.960911

$HO{-}CH_2{-}CH_2{-}OH$

E(RM062X) = -230.251965688

C	0.557076	0.510217	0.067275
H	0.458397	1.269099	-0.708997
H	0.493003	1.003145	1.039724
C	-0.557119	-0.510376	-0.066982
H	-0.492776	-1.003530	-1.039292
O	1.831173	-0.095542	-0.112724
H	1.984186	-0.696312	0.623715
O	-1.831194	0.095663	0.112417
H	-1.983557	0.696660	-0.623971
H	-0.458819	-1.269076	0.709515

$HO-CH_2-CH_2-OH\cdots H_2O$

E(RM062X) = -306.698522619

C	-0.948509	-0.807866	0.442230
H	-0.483597	-0.703668	1.426532
H	-1.840789	-1.422746	0.550517
C	-1.360849	0.549341	-0.069348
H	-2.152846	0.946889	0.569001
H	-1.737397	0.460421	-1.089778
O	-0.073040	-1.489675	-0.447865
H	-0.430692	2.216499	-0.538056
O	-0.225734	1.419553	-0.040283
H	1.520046	0.752991	0.043302
O	2.257150	0.120424	0.016448
H	0.806762	-1.092473	-0.361570
H	2.507652	-0.009182	0.936358

$HO-CH_2-CH_2-OH\cdots(H_2O)_2$

E(RM062X) = -383.141680198

O	-1.832498	0.906072	-0.207378
H	-2.529340	0.674800	0.416287
H	-0.263892	1.851672	0.291491
O	0.665792	2.097487	0.429850
H	0.831580	2.813559	-0.191391
H	1.684902	0.645527	-0.123300
O	0.268291	-2.075049	0.168023
O	2.214337	-0.115150	-0.427502
H	1.074656	-1.624547	-0.132582
H	2.949964	-0.170357	0.190237
C	-0.605386	-1.038474	0.589105
C	-1.162029	-0.288100	-0.608530
H	-0.342247	0.026111	-1.254670
H	-1.829897	-0.930259	-1.185381
H	-0.083514	-0.336584	1.245338
H	-1.415106	-1.497352	1.156586

$HO-CH_2-CH_2-OH\cdots(H_2O)_3$

E(RM062X) = -459.586259880

O	-1.760165	-1.071639	-0.727374
H	-2.134525	-1.872328	-0.343372
H	-2.121460	0.317456	0.400477
O	-2.182094	1.153636	0.898904
H	-1.842495	0.943861	1.774727
H	-0.758746	1.892191	0.030001
O	-0.017070	2.275228	-0.476303
H	-0.202120	2.045763	-1.392909
H	1.564861	1.467381	-0.207803
O	1.668483	-1.535163	0.512436
O	2.440234	1.036672	-0.145278

H	2.059715	-0.677315	0.264364
H	2.860706	1.429021	0.625899
C	0.266835	-1.331699	0.590316
C	-0.341846	-1.225814	-0.796204
H	0.041212	-0.343827	-1.310040
H	-0.083538	-2.109344	-1.382809
H	0.035894	-0.429960	1.166028
H	-0.164534	-2.187691	1.111689

$HO–CH_2–CH_2–OH\cdots(H_2O)_4$

E(RM062X) = -536.029098563

O	1.790852	-1.649198	-0.555540
H	1.936221	-2.170942	0.241489
H	0.055194	-1.578668	-1.148625
O	-0.880005	-1.447682	-1.389185
H	-1.010034	-0.492223	-1.355179
H	-1.479126	-1.737803	0.358681
O	-1.882112	-1.624914	1.238516
H	-1.137936	-1.512483	1.838828
H	-2.267344	0.116264	0.609146
O	-2.469142	0.946019	0.142056
H	-3.017758	0.678111	-0.602810
H	-1.037378	1.769794	-0.606614
O	1.414143	1.595324	1.126550
O	-0.267414	2.210720	-1.014056
H	0.938456	2.070387	0.424891
H	-0.535444	3.127187	-1.132525
C	1.178978	0.217825	0.878288
C	2.057158	-0.279084	-0.256268
H	1.840714	0.280901	-1.165787
H	3.110030	-0.139677	-0.004551
H	0.127405	0.046154	0.631748
H	1.409603	-0.331597	1.792448

Hydrolysis of 2-methyloxirane at 333 K. The nucleophilic substitution reaction occurs on the most substituted carbon atom.

H_2C-O-CH-$CH_3\cdots H_2O$

E(RM062X)=-269.532779306

C	0.24570	1.15687	-0.21986
C	0.73969	-0.21284	-0.35684
H	0.21679	-0.85710	-1.05465
O	-2.70892	-0.48440	-0.04088
H	-2.79924	0.10348	-0.79645
O	-0.07883	0.16183	0.76646
H	-1.82564	-0.29157	0.31376
H	-0.59721	1.48513	-0.81495
H	0.92336	1.92399	0.13161
C	2.15519	-0.57451	-0.03862

H	2.20923	-1.57822	0.38261
H	2.75489	-0.55589	-0.94866
H	2.57633	0.13363	0.67402

H_2C-O-CH-$CH_3\cdots(H_2O)_2$

E(RM062X)=-345.975892269

C	1.60978	-1.15372	0.20269
H	2.61504	-1.18332	-0.19741
C	0.95542	0.14335	0.37009
H	0.16093	0.20048	1.10709
O	0.61583	-0.71197	-0.73755
H	-1.36132	1.88755	0.30323
O	-2.14465	1.50372	-0.10129
H	-2.07548	0.54975	0.07223
O	-1.92740	-1.31898	0.23245
H	-1.06977	-1.29076	-0.22577
H	-2.53301	-1.73271	-0.39022
C	1.63386	1.42900	0.01971
H	0.91426	2.14477	-0.37939
H	2.08535	1.86236	0.91207
H	2.41399	1.25980	-0.72149
H	1.30541	-1.99182	0.81580

H_2C-O-CH-$CH_3\cdots(H_2O)_3$

E(RM062X)=-422.420655826

O	0.22270	2.72930	0.15690
H	-0.56610	2.33530	0.54060
H	0.86500	2.00060	0.08910
O	2.29210	0.83550	-0.11790
H	2.68810	1.08810	-0.95780
H	2.06270	-0.10730	-0.22070
O	-0.94510	-1.53300	0.31790
O	1.74430	-1.90740	-0.37470
H	0.80770	-1.98370	-0.12440
H	2.23090	-2.29750	0.35850
C	-0.71680	-0.37040	1.13470
C	-1.04150	-0.23000	-0.28550
H	0.30740	-0.25330	1.46690
H	-1.49090	-0.18530	1.86830
H	-0.21690	-0.02110	-0.95900
C	-2.40340	0.18830	-0.74060
H	-2.41570	1.26500	-0.91370
H	-2.66610	-0.30970	-1.67360
H	-3.14820	-0.05460	0.01630

H_2C-O-CH-$CH_3\cdots(H_2O)_4$

E(RM062X)=-498.864386909

O	2.90620	0.39030	-0.26440
H	2.49300	1.10960	0.22200

H	2.50250	-0.42250	0.09140
O	1.83400	-2.03710	0.62530
H	1.54820	-1.87000	1.52900
H	1.00930	-2.09010	0.10340
O	-0.40220	-2.18290	-1.01950
H	-0.13070	-1.64320	-1.76900
H	-1.20210	-1.74520	-0.67060
O	-1.42270	1.30720	0.71950
O	-2.76870	-1.02710	-0.04780
H	-2.48270	-0.16930	0.31030
H	-3.03880	-1.54200	0.71930
C	-0.17670	0.64750	1.00510
C	-0.41390	1.25030	-0.30700
H	-0.68010	0.57820	-1.11590
H	-0.26620	-0.42400	1.12910
C	0.18950	2.56340	-0.69450
H	1.08730	2.39730	-1.28980
H	-0.51170	3.14290	-1.29490
H	0.45510	3.13670	0.19310
H	0.45160	1.17090	1.71540

H_2C-O-CH-$CH_3\cdots(H_2O)_5$

E(RM062X)=-575.310349386

O	1.07630	-2.63100	-0.38160
H	1.36480	-2.19690	0.42690
H	0.43020	-2.02090	-0.77810
O	-1.02190	-1.09450	-1.53100
H	-0.91820	-0.12970	-1.50060
H	-1.51770	-1.31160	-0.72230
O	-2.20790	-1.62490	0.99580
H	-1.38230	-1.72620	1.48060
H	-2.40820	-0.66970	1.03020
O	-2.76160	1.09460	0.76670
H	-3.65310	1.14150	0.40710
H	-2.17850	1.37090	0.03710
O	1.26070	1.68730	0.45600
O	-0.91580	1.75410	-1.25680
H	-0.12180	2.01970	-0.76180
H	-1.07220	2.44090	-1.91240
C	0.77800	0.44480	0.99850
C	1.79990	0.45280	-0.04980
H	1.46660	0.23610	-1.05930
H	-0.25010	0.21690	0.74390
H	1.07910	0.26010	2.02190
C	3.24090	0.19040	0.25360
H	3.46700	-0.86130	0.07530
H	3.88310	0.79070	-0.39060
H	3.45970	0.42630	1.29440

$[H_2C\text{-}O\text{-}CH\text{-}CH_3\cdots H_2O]^{\ddagger}$

E(RM062X)=-269.460708825

C	-0.34666	1.22429	0.38281
C	-0.67531	-0.20457	0.58422
H	-0.37339	-0.72066	1.48871
O	1.66866	-1.00855	0.00588
H	2.18673	-0.84320	0.79937
O	0.58353	1.15920	-0.66543
H	1.38248	-0.08672	-0.33134
H	0.05130	1.67135	1.29714
H	-1.27130	1.75151	0.10639
C	-1.45243	-0.94591	-0.37401
H	-1.12322	-1.97744	-0.48388
H	-2.42275	-1.01105	0.15945
H	-1.60104	-0.43184	-1.31754

$[H_2C\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_2]^{\ddagger}$

E(RM062X)=-345.904074202

C	0.48932	-1.24052	0.52578
H	1.23808	-2.04764	0.52991
C	1.20076	0.05137	0.55037
H	1.01582	0.77013	1.33854
O	-0.23183	-1.14800	-0.67080
H	-0.65910	2.35892	0.74501
O	-0.62567	1.83422	-0.06099
H	-1.36757	1.20382	0.01555
O	-2.45099	-0.25425	0.07524
H	-1.57175	-0.67082	-0.27915
H	-3.05503	-0.23865	-0.67213
C	2.21406	0.37708	-0.41905
H	2.18033	1.41898	-0.73365
H	3.12888	0.30103	0.20214
H	2.27972	-0.32225	-1.24510
H	-0.14624	-1.35686	1.40863

$[H_2C\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_3]^{\ddagger}$

E(RM062X)=-422.370949761

O	-0.85090	1.90060	0.10800
H	-1.21000	2.02510	0.99520
H	0.12700	1.95360	0.19590
O	1.87230	1.59160	0.07080
H	2.23850	2.07160	-0.67860
H	1.98230	0.64500	-0.15330
O	-0.23090	-1.87070	0.27880
O	2.13710	-1.14730	-0.54020
H	1.26090	-1.53450	-0.23620
H	2.79580	-1.47640	0.07840
C	-0.43130	-0.68480	1.01180
C	-0.89210	-0.08120	-0.23580

H	0.48060	-0.25150	1.43060
H	-1.20500	-0.75610	1.77980
H	-0.13290	0.07570	-0.98720
C	-2.30710	-0.20230	-0.67430
H	-2.51070	0.48810	-1.48860
H	-2.47910	-1.21350	-1.04110
H	-2.98500	-0.01190	0.15600

$[H_2C\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_4]^{\ddagger}$

E(RM062X)=-498.816887381

O	-1.05150	1.87510	-0.41200
H	-1.74700	2.17770	0.18500
H	-0.19710	2.10200	0.03150
O	1.37160	2.32580	0.66440
H	1.30560	2.07760	1.59210
H	1.77580	1.55080	0.21900
O	2.41550	0.25880	-0.79170
H	2.08740	0.44070	-1.67800
H	2.10060	-0.64920	-0.58040
O	-0.75020	-1.79230	0.66370
O	1.58060	-2.26490	-0.22120
H	0.64190	-2.12190	0.15540
H	2.11540	-2.57430	0.51560
C	-0.67010	-0.43940	1.05010
C	-1.14310	-0.12810	-0.29400
H	-0.40620	-0.22060	-1.08020
H	0.34380	-0.09730	1.27260
C	-2.58200	-0.24770	-0.65940
H	-2.80690	0.41460	-1.49220
H	-2.79080	-1.26500	-0.98420
H	-3.22010	-0.00560	0.18920
H	-1.35910	-0.15880	1.84950

$[H_2C\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_5]^{\ddagger}$

E(RM062X)=-575.259420558

O	1.50450	-1.84570	-0.63200
H	1.58610	-2.32440	0.20210
H	0.54320	-1.85490	-0.85650
O	-1.11970	-1.64940	-1.24830
H	-1.20700	-0.71550	-1.47450
H	-1.51940	-1.71640	-0.36100
O	-2.29030	-1.52260	1.32080
H	-1.53320	-1.42580	1.90700
H	-2.49060	-0.61730	1.01310
O	-2.90190	0.84270	0.00480
H	-3.25820	0.40760	-0.77650
H	-2.12100	1.34290	-0.31980
O	1.08130	1.70230	0.75240
O	-0.76680	2.28270	-0.91590

H	-0.01220	2.14120	-0.25050
H	-1.01820	3.20730	-0.83640
C	0.75320	0.33940	0.89680
C	1.74000	0.08930	-0.14830
H	1.43800	0.36520	-1.14870
H	-0.27740	0.09820	0.62510
H	1.00600	-0.08600	1.87080
C	3.19440	0.01630	0.16050
H	3.72140	-0.49130	-0.64340
H	3.59860	1.02370	0.23920
H	3.36220	-0.50450	1.10210

$HO\text{-}H_2C\text{-}CHOH\text{-}CH_3$

E(RM062X)=-269.564894978

C	-0.94047	-0.05446	0.66995
C	0.55609	0.10322	0.46833
H	1.00784	0.25440	1.45267
O	0.81181	1.24646	-0.35669
H	0.48219	2.02817	0.09960
O	-1.63028	-0.27425	-0.55432
H	-1.36900	0.42811	-1.16027
H	-1.33062	0.83894	1.16687
H	-1.13855	-0.91590	1.30656
C	1.19166	-1.08956	-0.21129
H	2.26689	-0.94371	-0.30454
H	1.01336	-1.99216	0.37231
H	0.77192	-1.23071	-1.20702

$HO\text{-}H_2C\text{-}CHOH\text{-}CH_3\cdots H_2O$

E(RM062X)=-346.009618288

C	0.86899	1.08834	-0.47913
H	1.78884	1.59469	-0.18698
C	1.05835	-0.40811	-0.28740
H	1.99710	-0.67762	-0.77845
O	-0.16984	1.65066	0.31040
H	-0.02636	-0.93292	-1.84478
O	-0.00839	-1.14879	-0.90548
H	-1.65966	-0.70965	-0.20620
O	-2.41872	-0.20470	0.13615
H	-0.98459	1.14509	0.17186
H	-2.48061	-0.45014	1.06456
C	1.09505	-0.82291	1.16669
H	1.30968	-1.88715	1.25159
H	1.86826	-0.26826	1.69731
H	0.13446	-0.62335	1.64265
H	0.69417	1.28814	-1.54110

$HO\text{-}H_2C\text{-}CHOH\text{-}CH_3\cdots(H_2O)_2$

E(RM062X)=-422.453270151

O	-0.85390	1.64220	0.17620
H	-1.43010	1.76550	0.93970
H	1.02060	1.76300	0.26810
O	1.97450	1.59020	0.19480
H	2.27380	2.13990	-0.53630
H	2.10810	-0.16570	-0.36770
O	-0.25620	-1.95690	0.44770
O	2.18030	-1.09050	-0.67030
H	0.59080	-1.90480	-0.02580
H	2.93020	-1.45260	-0.18840
C	-0.51500	-0.63750	0.90190
C	-0.94040	0.27420	-0.24310
H	0.37310	-0.21830	1.38200
H	-1.31330	-0.69330	1.64490
H	-0.20560	0.17800	-1.04540
C	-2.32560	-0.05120	-0.75960
H	-2.57940	0.57960	-1.61050
H	-2.37750	-1.09360	-1.07350
H	-3.06240	0.10870	0.03030

HO-H_2C-CHOH-$CH_3$$\cdots$$(H_2O)_3$

E(RM062X)=-498.897556313

O	-0.87500	1.72380	-0.25740
H	-1.57730	2.10090	0.28680
H	0.72420	2.05940	0.53330
O	1.65250	2.14140	0.82360
H	1.67720	1.72390	1.69040
H	2.16360	0.82160	-0.33150
O	2.38740	0.13710	-0.99020
H	1.85470	0.35700	-1.76160
H	1.77730	-1.47380	-0.46180
O	-0.99490	-1.75120	0.92090
O	1.44580	-2.36430	-0.23230
H	-0.18150	-2.08470	0.49970
H	2.01440	-2.66800	0.48210
C	-0.86980	-0.34030	0.97610
C	-1.11440	0.31420	-0.37800
H	-0.36600	-0.04810	-1.08580
H	0.12410	-0.05710	1.33640
C	-2.50770	0.05450	-0.91030
H	-2.64270	0.53370	-1.87920
H	-2.68250	-1.01390	-1.02710
H	-3.25020	0.45230	-0.21450
H	-1.60940	0.03270	1.68870

HO-H_2C-CHOH-$CH_3$$\cdots$$(H_2O)_4$

E(RM062X)=-575.340465994

O	1.44870	-1.55250	-0.62020
H	1.61720	-2.10480	0.15280

H	-0.29580	-1.54460	-1.17550
O	-1.24220	-1.48150	-1.40140
H	-1.43590	-0.53670	-1.38120
H	-1.78490	-1.78210	0.36810
O	-2.15870	-1.68040	1.26210
H	-1.39580	-1.55310	1.83520
H	-2.60360	0.05620	0.67750
O	-2.83830	0.89570	0.24420
H	-3.44710	0.64530	-0.45860
H	-1.47520	1.70800	-0.62460
O	0.95100	1.65130	1.09720
O	-0.72920	2.13830	-1.08510
H	0.46430	2.09470	0.38300
H	-1.03510	3.02850	-1.28360
C	0.82560	0.26180	0.83840
C	1.75570	-0.19390	-0.27940
H	1.52720	0.38280	-1.17760
H	-0.20550	0.01810	0.56820
H	1.07570	-0.27330	1.75790
C	3.21800	-0.04680	0.08290
H	3.85110	-0.35360	-0.74860
H	3.44720	0.98910	0.32980
H	3.44970	-0.66870	0.95050

Hydrolysis of 2-methyloxirane at 333 K. The nucleophilic substitution reaction occurs on the least substituted carbon atom.

H_2C-O-CH-CH_3···H_2O

E(RM062X)=-269.532610298

C	-0.33829	1.19832	0.27471
H	-1.06739	1.91943	-0.07163
H	0.45811	1.57322	0.90423
C	-0.72288	-0.21029	0.35263
H	-0.16682	-0.83482	1.04277
O	2.64825	-0.51741	0.14460
H	3.32766	0.02217	-0.26930
O	0.09115	0.26832	-0.73444
H	1.81439	-0.21768	-0.25356
C	-2.09690	-0.67185	-0.01520
H	-2.06095	-1.66598	-0.46018
H	-2.72113	-0.72088	0.87707
H	-2.55063	0.02023	-0.72354

H_2C-O-CH-CH_3···$(H_2O)_2$

E(RM062X)=-345.975013203

C	-1.48670	0.20150	-0.30200
H	-1.25900	1.10750	-0.85310
C	-0.54080	-0.90610	-0.43120
H	0.32670	-0.79880	-1.06990

H	-0.88750	-1.91460	-0.24630
O	-0.52440	-0.06580	0.73650
H	3.01070	-1.22180	0.85740
O	3.07550	-0.89940	-0.04600
H	2.60770	-0.04710	-0.03800
O	1.63190	1.54780	-0.00510
H	0.85540	1.08600	0.35770
H	1.40530	1.71950	-0.92480
C	-2.91900	-0.02220	0.06350
H	-3.28810	0.79440	0.68360
H	-3.52790	-0.06530	-0.83950
H	-3.02910	-0.95980	0.60700

H_2C-O-CH-$CH_3\cdots(H_2O)_3$

E(RM062X)=-422.420613284

O	-0.38970	2.71650	0.27690
H	0.49350	2.47490	-0.01710
H	-0.95460	1.96140	0.03460
O	-2.26300	0.72200	-0.42260
H	-2.99930	0.89700	0.17160
H	-2.03980	-0.21690	-0.28040
O	1.01240	-1.45680	0.42290
O	-1.68050	-2.01410	-0.10800
H	-0.71930	-2.02310	0.03950
H	-1.80170	-2.36370	-0.99650
C	1.05620	-0.21670	-0.30790
C	0.70530	-0.23050	1.11120
H	-0.33110	-0.13240	1.40960
H	1.45120	0.07170	1.83520
C	2.40540	0.22650	-0.77710
H	2.37190	1.28580	-1.03620
H	3.14700	0.08110	0.00740
H	2.70750	-0.33110	-1.66320
H	0.23920	-0.12190	-1.01560

H_2C-O-CH-$CH_3\cdots(H_2O)_4$

E(RM062X)=-498.865697538

O	2.91190	0.43110	1.00750
H	2.73730	-0.51110	0.92850
H	2.31190	0.85380	0.36640
O	1.34180	1.87050	-0.81630
H	1.32500	1.33210	-1.61420
H	0.41020	1.93120	-0.52980
O	-1.28550	2.21980	0.06700
H	-1.16840	2.42940	0.99910
H	-1.86180	1.43230	0.05860
O	-0.93070	-1.80160	0.28980
O	-3.04570	0.02470	0.07120
H	-2.46590	-0.75540	0.09750

H	-3.46820	-0.00390	-0.79280
C	0.01420	-0.98330	-0.42550
C	-0.10350	-0.88360	1.02860
H	-0.63850	-0.05290	1.47230
H	0.64290	-1.36600	1.64680
H	-0.47260	-0.21170	-1.01230
C	1.15320	-1.70120	-1.07720
H	0.81960	-2.21120	-1.98070
H	1.92530	-0.98250	-1.35630
H	1.58470	-2.43190	-0.39330

H_2C-O-CH-$CH_3\cdots(H_2O)_5$

E(RM062X)=-575.309269492

O	-3.36400	0.00930	-0.87760
H	-3.21990	-0.73050	-0.28060
H	-2.54210	0.53010	-0.84060
O	-1.12290	1.70450	-1.04680
H	-0.46460	1.16580	-1.49840
H	-0.70320	1.94620	-0.20130
O	0.32770	2.45290	1.26730
H	0.15930	1.80580	1.95990
H	1.10460	2.11460	0.78400
O	2.31980	1.56510	-0.49240
H	1.83990	1.74340	-1.30780
H	2.49480	0.60500	-0.50600
O	0.40830	-2.17120	0.36480
O	2.87810	-1.18580	-0.54850
H	2.11900	-1.66320	-0.17190
H	3.60270	-1.34140	0.06540
C	-0.18080	-0.86880	0.54360
C	-0.41900	-1.63000	-0.68160
H	0.11690	-1.37090	-1.58670
H	-1.36510	-2.14100	-0.80580
H	0.55620	-0.07590	0.48790
C	-1.21070	-0.74550	1.62040
H	-0.73790	-0.73760	2.60290
H	-1.75640	0.19150	1.49800
H	-1.91720	-1.57450	1.57170

$[H_2C$-O-CH-$CH_3\cdots H_2O]^{\ddagger}$

E(RM062X)=-269.445923659

C	0.20651	1.00393	-0.06240
H	0.27721	1.14740	-1.13332
H	0.75337	1.67990	0.57795
C	-0.70193	-0.03628	0.41492
H	-0.73830	-0.06267	1.50767
O	2.28242	-0.00644	0.07701
H	2.61545	0.12389	-0.81722
O	0.02924	-1.10760	-0.12896

H	1.53704	-0.67907	-0.00963
C	-2.10379	0.09412	-0.15685
H	-2.66309	-0.80169	0.11513
H	-2.62083	0.96584	0.24421
H	-2.05885	0.16800	-1.24327

$[H_2C\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_2]^{\ddagger}$
E(RM062X)=-345.8919384

C	1.01540	-0.19940	-0.27780
H	0.77860	-0.77590	-1.17860
C	0.49830	1.16170	-0.37380
H	0.03100	1.57180	-1.25570
H	0.70610	1.83060	0.45090
O	0.22990	-0.58280	0.82000
H	-1.70310	1.38990	1.05610
O	-1.75800	1.35790	0.09430
H	-2.00610	0.43410	-0.10160
O	-1.94550	-1.41550	-0.20090
H	-1.04900	-1.16270	0.21470
H	-1.74530	-1.70260	-1.09620
C	2.51180	-0.23990	-0.01150
H	2.78360	-1.27540	0.19830
H	3.08390	0.10620	-0.87230

$[H_2C\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_3]^{\ddagger}$
E(RM062X)=-422.372034534

O	-0.02590	2.12120	-0.51610
H	-0.67560	2.45520	0.11640
H	0.78060	1.90140	0.00330
O	2.14230	0.94630	0.67370
H	2.96940	1.22330	0.26660
H	2.03360	0.00980	0.41920
O	-0.90800	-1.51940	-0.50960
O	1.71600	-1.78790	-0.10980
H	0.73730	-1.82100	-0.28550
H	1.84480	-2.28770	0.70180
C	-0.92980	-0.36450	0.29950
C	-0.49830	0.31710	-0.91840
H	0.49760	0.13390	-1.28710
H	-1.26250	0.55580	-1.64350
C	-2.28450	0.01490	0.84530
H	-2.24150	0.98760	1.33870
H	-3.01770	0.05850	0.03910
H	-2.61130	-0.72480	1.57640
H	-0.17400	-0.37820	1.09070

$[H_2C\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_4]^{\ddagger}$
E(RM062X)=-498.820105686

O	1.66170	1.07690	1.22210

H	2.55520	0.81820	0.96350
H	1.31350	1.63110	0.47300
O	0.52240	2.39310	-0.76950
H	0.80760	1.91770	-1.55740
H	-0.38970	2.07530	-0.59590
O	-2.02660	1.59040	-0.15610
H	-2.21630	1.98580	0.70030
H	-2.20420	0.63030	-0.04230
O	-0.18810	-2.01190	0.14520
O	-2.56570	-1.07210	0.14350
H	-1.64770	-1.50450	0.12720
H	-2.99730	-1.34320	-0.67170
C	0.55020	-0.92790	-0.37750
C	0.62050	-0.52870	1.02490
H	-0.25380	-0.07760	1.46890
H	1.28720	-1.08790	1.66170
H	-0.06200	-0.26390	-0.99410
C	1.84290	-1.28730	-1.06370
H	1.63710	-1.83490	-1.98370
H	2.40070	-0.38450	-1.32010
H	2.45870	-1.91030	-0.41370

$[H_2C\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_5]^{\ddagger}$

E(RM062X)=-575.263173413

O	2.15030	-1.14720	-1.18100
H	2.63910	-1.52970	-0.44150
H	1.25790	-1.58350	-1.17310
O	-0.33060	-2.09760	-1.19650
H	-0.79230	-1.37400	-1.63630
H	-0.66240	-2.07110	-0.27850
O	-1.54370	-1.85390	1.33200
H	-0.93670	-1.47140	1.97390
H	-1.99960	-1.09160	0.92430
O	-2.81190	0.10080	-0.18000
H	-2.88250	-0.38760	-1.00650
H	-2.26960	0.89000	-0.39470
O	0.87610	1.98330	0.45640
O	-1.33770	2.33640	-0.80110
H	-0.46420	2.28170	-0.29380
H	-1.80270	3.09590	-0.43910
C	0.82530	0.57640	0.55660
C	1.69250	0.63270	-0.61470
H	1.24380	0.86630	-1.56740
H	2.72340	0.90660	-0.45340
H	-0.16930	0.17680	0.34210
C	1.39640	-0.01080	1.82190
H	0.77040	0.25870	2.67380
H	1.43600	-1.10040	1.75470
H	2.40430	0.36840	1.99450

HO-H_2C-CHOH-CH_3

E(RM062X)=-269.565177814

C	0.71907	-0.70834	0.21494
H	0.63828	-0.75983	1.30392
H	0.72403	-1.72265	-0.19053
C	-0.46343	0.05252	-0.34008
H	-0.36178	0.10679	-1.42867
O	1.90311	-0.00904	-0.16219
H	2.64992	-0.39630	0.30341
O	-0.48507	1.37953	0.19064
H	0.37933	1.77212	0.02501
C	-1.76952	-0.61417	0.02610
H	-2.60935	-0.04825	-0.37422
H	-1.80835	-1.62310	-0.38275
H	-1.87308	-0.67277	1.11046

HO-H_2C-CHOH-CH_3···H_2O

E(RM062X)=-346.009249197

C	-0.82150	-0.23330	0.26460
H	-0.43040	-0.39880	1.27370
C	-0.52320	1.19570	-0.13780
H	-1.09370	1.87660	0.49740
H	-0.82080	1.34550	-1.17810
O	-0.20460	-1.15830	-0.63120
H	1.09200	2.27960	-0.41230
O	0.87560	1.44560	0.01480
H	2.16480	0.08940	0.17770
O	2.54780	-0.80190	0.13440
H	0.74600	-1.17530	-0.44230
H	2.60530	-1.09320	1.04960
C	-2.31390	-0.48740	0.23950
H	-2.52560	-1.51780	0.52030
H	-2.82760	0.17470	0.93490
H	-2.70820	-0.31280	-0.76280

HO-H_2C-CHOH-CH_3···$(H_2O)_2$

E(RM062X)=-422.453406985

O	-0.29060	-1.91600	0.46270
H	-1.08440	-2.27880	0.05590
H	1.33450	-1.54110	-0.40780
O	2.14320	-1.10290	-0.72140
H	2.86220	-1.52990	-0.24490
H	2.05280	0.64130	-0.10060
O	-0.82220	1.69660	0.23650
O	2.00250	1.55140	0.24710
H	0.12670	1.87320	0.35020
H	2.35290	2.10640	-0.45640
C	-0.91380	0.35280	-0.22970

C	-0.55630	-0.58920	0.91480
H	0.36370	-0.24520	1.38740
H	-1.35430	-0.58830	1.66190
C	-2.31630	0.12500	-0.74800
H	-2.43970	-0.90210	-1.09330
H	-3.04100	0.31290	0.04590
H	-2.52880	0.79030	-1.58400
H	-0.18940	0.19740	-1.03600

$HO\text{-}H_2C\text{-}CHOH\text{-}CH_3\cdots(H_2O)_3$

E(RM062X)=-498.898227575

O	1.04550	1.02070	1.32460
H	2.00760	1.01620	1.36200
H	0.79630	1.99190	-0.25100
O	0.44330	2.44830	-1.03540
H	0.70200	1.89110	-1.77690
H	-1.21940	1.78310	-0.40630
O	-2.00520	1.47380	0.07660
H	-1.76370	1.56170	1.00480
H	-2.29350	-0.32400	-0.07410
O	0.15080	-2.16270	-0.27340
O	-2.50050	-1.27800	-0.08670
H	-0.81440	-2.06660	-0.19960
H	-2.98220	-1.41940	-0.90750
C	0.68300	-0.84100	-0.23470
C	0.59290	-0.32850	1.19780
H	-0.44690	-0.34350	1.52460
H	1.17270	-0.98300	1.85270
H	0.07740	-0.19170	-0.87480
C	2.10670	-0.87660	-0.74390
H	2.13640	-1.24960	-1.76690
H	2.54360	0.12240	-0.73390
H	2.71610	-1.52790	-0.11430

$HO\text{-}H_2C\text{-}CHOH\text{-}CH_3\cdots(H_2O)_4$

E(RM062X)=-575.34136943

O	1.85370	-0.98650	-1.33130
H	2.40700	-1.54290	-0.77250
H	0.19200	-1.74820	-1.27020
O	-0.68760	-2.16470	-1.20830
H	-1.28450	-1.54740	-1.64430
H	-1.19640	-1.94540	0.52240
O	-1.63940	-1.72290	1.36430
H	-0.93770	-1.40330	1.94030
H	-2.36930	-0.25210	0.48420
O	-2.75810	0.43980	-0.08130
H	-2.95510	-0.00460	-0.91240
H	-1.66020	1.81210	-0.52340
O	0.99020	1.78950	0.90950

O	-1.07480	2.54290	-0.80100
H	0.34340	2.25000	0.34680
H	-1.51790	3.34550	-0.50910
C	0.99470	0.43080	0.48020
C	1.83560	0.33310	-0.78650
H	1.41210	0.97930	-1.55460
H	2.85360	0.66740	-0.57160
H	-0.02970	0.12250	0.24450
C	1.54140	-0.42850	1.59900
H	0.94890	-0.29690	2.50510
H	1.51780	-1.48410	1.32400
H	2.57380	-0.14900	1.81930

Hydrolysis of 2,2-dimethyloxirane at 333 K. The substitution reaction occurs on the most substituted carbon atom

H_2C-O-C-$(CH_3)_2\cdots H_2O$

E(RM062X)=-308.845518519

C	-0.78650	0.09280	-0.10100
C	-0.32320	-1.07590	-0.85220
H	-0.96280	-1.94530	-0.93380
O	2.87210	0.01010	0.31950
H	2.82920	0.91310	-0.00800
O	0.16770	-0.82560	0.47770
H	1.94560	-0.27620	0.37370
H	0.41750	-0.94470	-1.63160
C	-2.13710	0.06420	0.55460
H	-2.12250	0.64820	1.47590
H	-2.88050	0.50110	-0.11250
H	-2.43090	-0.95830	0.78630
C	-0.22570	1.45130	-0.41190
H	-0.08100	2.01470	0.51130
H	0.72600	1.37200	-0.93500
H	-0.92420	2.00420	-1.04020

H_2C-O-C-$(CH_3)_2\cdots(H_2O)_3$

E(RM062X)=-461.733375615

O	-1.36250	2.54030	-0.27290
H	-0.41650	2.36830	-0.27780
H	-1.77700	1.66460	-0.17470
O	-2.81340	0.13710	-0.03550
H	-3.28100	0.24800	0.79820
H	-2.30130	-0.68730	0.07010
O	1.13090	-1.22990	-0.50310
O	-1.38060	-2.24840	0.24930
H	-0.47220	-1.99410	0.00890
H	-1.67660	-2.82540	-0.46190
C	0.68430	-0.03770	-1.17630
C	1.40040	0.05570	0.10000

H	-0.39290	0.08060	-1.19250
H	1.20930	0.17820	-2.09810
C	0.64200	0.31710	1.37080
H	1.09100	-0.24230	2.19290
H	0.69090	1.37830	1.61810
H	-0.40390	0.02930	1.27050
C	2.85370	0.43330	0.10580
H	3.32480	0.17360	-0.84060
H	2.95530	1.50670	0.26750
H	3.37150	-0.08220	0.91580

H_2C-O-C-$(CH_3)_2\cdots(H_2O)_4$

E(RM062X)=-538.177783201

O	2.49460	1.88000	-0.32480
H	2.57420	1.08030	-0.85260
H	1.54060	1.99120	-0.16600
O	-0.15080	2.59840	0.24990
H	-0.24800	3.40750	-0.26200
H	-0.97190	2.09600	0.08570
O	-2.60580	1.35180	-0.19330
H	-3.14330	1.70490	0.52260
H	-2.63140	0.38190	-0.07490
O	-0.03100	-1.84300	-0.58270
O	-2.68950	-1.40850	0.11470
H	-1.77530	-1.65070	-0.12260
H	-3.23610	-1.76000	-0.59510
C	0.36610	-0.57470	-1.13740
C	0.87850	-1.00610	0.16740
H	-0.43010	0.15980	-1.17650
H	1.00000	-0.65030	-2.01230
C	0.29800	-0.42110	1.42350
H	0.23760	-1.18650	2.19870
H	0.94360	0.37990	1.78500
H	-0.69610	-0.01330	1.24350
C	2.26600	-1.57100	0.27620
H	2.96010	-0.79390	0.59690
H	2.28500	-2.36860	1.02040
H	2.59880	-1.96990	-0.68070

H_2C-O-C-$(CH_3)_2\cdots(H_2O)_5$

E(RM062X)=-614.621961149

O	2.38600	-2.37200	0.03180
H	2.49840	-1.74650	0.75330
H	1.45560	-2.28230	-0.24340
O	-0.24560	-2.30580	-0.92080
H	-0.35230	-1.43790	-1.32500
H	-0.86060	-2.29720	-0.16460
O	-2.20210	-2.08100	1.10300
H	-1.76810	-1.71650	1.88080

H	-2.48340	-1.30510	0.58000
O	-2.85300	-0.05920	-0.68430
H	-2.38820	-0.31650	-1.48720
H	-2.51420	0.83050	-0.46320
O	0.56950	1.73410	0.93540
O	-1.94790	2.47790	-0.01030
H	-1.06290	2.30170	0.35800
H	-2.47620	2.78550	0.73310
C	0.50950	0.29660	1.01310
C	1.30750	0.94930	-0.02910
H	-0.45660	-0.11670	0.74790
H	0.99930	-0.12460	1.88250
C	0.77010	1.01260	-1.43090
H	1.05700	1.95160	-1.90610
H	1.18920	0.19410	-2.01870
H	-0.31770	0.93030	-1.43520
C	2.79770	1.06170	0.11820
H	3.09060	0.98110	1.16400
H	3.29020	0.27260	-0.44940
H	3.13680	2.02210	-0.27280

$[H_2C\text{-}O\text{-}C\text{-}(CH_3)_2\cdots H_2O]^{\ddagger}$

E(RM062X)=-308.790330646

C	-0.56134	-0.23133	-0.09935
C	0.61539	-1.06489	0.23831
H	0.58348	-1.26969	1.31909
O	0.67389	1.46240	0.74326
H	0.58251	2.19752	0.12859
O	1.81842	-0.57891	-0.20919
H	1.37093	0.83796	0.33857
H	0.28999	-2.02340	-0.23492
C	-1.76765	-0.31566	0.73593
H	-1.91035	0.66646	1.19575
H	-2.64321	-0.49317	0.11051
H	-1.67521	-1.06399	1.51902
C	-0.67463	0.38143	-1.42874
H	-1.35791	1.22815	-1.42319
H	0.28857	0.63612	-1.85754
H	-1.13794	-0.40121	-2.04542

$[H_2C\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_3]^{\ddagger}$

E(RM062X)=-461.68062002

O	0.91970	1.96670	-0.44690
H	1.08960	1.97330	-1.39610
H	-0.05370	1.98180	-0.36390
O	-1.91830	1.73420	-0.12000
H	-2.12090	2.14620	0.72590
H	-2.13290	0.78960	0.00400
O	-0.09060	-1.93700	-0.42000

O	-2.44510	-1.06650	0.24090
H	-1.56120	-1.49920	0.00560
H	-3.06360	-1.35310	-0.43720
C	0.27740	-0.70750	-0.97960
C	1.07680	-0.21700	0.16790
H	-0.57130	-0.05740	-1.20760
H	0.89950	-0.79600	-1.87670
C	0.45440	0.02640	1.48410
H	0.76710	-0.77990	2.15260
H	0.86980	0.94440	1.90010
H	-0.62760	0.07230	1.44580
C	2.53890	-0.37280	0.11680
H	2.93430	-0.00030	-0.82660
H	3.03650	0.07800	0.97110
H	2.72280	-1.45340	0.13630

$[H_2C\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_4]^{\ddagger}$

E(RM062X)=-538.13148138

O	1.47010	1.87780	-0.08260
H	1.84160	1.97100	-0.96780
H	0.52630	2.14990	-0.16030
O	-1.15680	2.54550	-0.13420
H	-1.37850	2.97400	-0.96690
H	-1.72010	1.74500	-0.09960
O	-2.87690	0.39310	0.00810
H	-3.36920	0.54700	0.82050
H	-2.47660	-0.49960	0.11400
O	0.47080	-1.87200	-0.78960
O	-1.81520	-2.10420	0.26470
H	-0.88520	-2.05360	-0.16840
H	-2.34730	-2.64660	-0.32480
C	0.54340	-0.50000	-1.08720
C	1.26260	-0.23770	0.16530
H	-0.43240	-0.00470	-1.13600
H	1.12850	-0.26770	-1.98090
C	0.50160	-0.14290	1.43950
H	0.48770	-1.12700	1.90990
H	1.01770	0.53240	2.11940
H	-0.52040	0.19180	1.27490
C	2.71860	-0.52270	0.24490
H	3.18480	0.16900	0.94370
H	2.85510	-1.52750	0.64610
H	3.19460	-0.45480	-0.73050

$[H_2C\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_5]^{\ddagger}$

E(RM062X)=-614.574810415

O	1.40770	-2.10130	-0.09540
H	1.58840	-2.36690	0.81390
H	0.44000	-2.23430	-0.22390

O	-1.23910	-2.38450	-0.58960
H	-1.36740	-1.81650	-1.35720
H	-1.75360	-1.95890	0.12260
O	-2.80440	-0.99080	1.27310
H	-2.22980	-0.70880	1.99170
H	-2.76290	-0.26850	0.61260
O	-2.67930	0.81640	-0.79100
H	-2.39310	0.30790	-1.55650
H	-1.97540	1.49180	-0.64780
O	1.00800	1.65900	1.01720
O	-0.81140	2.71680	-0.36730
H	-0.06840	2.30040	0.21150
H	-1.23490	3.37910	0.18660
C	0.74320	0.28130	1.10170
C	1.59920	0.02110	-0.06210
H	-0.30620	0.01740	0.92590
H	1.10100	-0.18340	2.02410
C	1.04480	0.24430	-1.42370
H	1.36970	1.22230	-1.78160
H	1.45450	-0.49800	-2.10670
H	-0.04270	0.20060	-1.42560
C	3.07710	0.00870	0.09740
H	3.36870	-0.28810	1.10220
H	3.51640	-0.66270	-0.63760
H	3.45820	1.00900	-0.10850

HO-H_2C-COH-$(CH_3)_2$

E(RM062X)=-308.87574531

C	-0.39370	0.00010	0.00880
C	0.86830	-0.74150	-0.40750
H	0.88270	-1.71650	0.08820
O	-0.26540	0.16410	1.43140
H	-0.98280	0.73180	1.73310
O	2.05400	-0.01980	-0.10260
H	2.00960	0.21770	0.83040
H	0.85860	-0.89890	-1.48500
C	-1.61020	-0.85590	-0.30700
H	-2.51520	-0.35940	0.04530
H	-1.70080	-1.01240	-1.38230
H	-1.53120	-1.82650	0.18330
C	-0.49170	1.36400	-0.65720
H	-1.39040	1.87930	-0.31400
H	0.37540	1.97570	-0.41190
H	-0.55070	1.25470	-1.74030

HO-H_2C-COH-$(CH_3)_2\cdots(H_2O)_2$

E(RM062X)=-461.765870051

O	0.21760	0.51310	-1.05050
H	-0.01390	-0.21110	-1.64480

H	-1.23060	1.31490	-0.28770
O	-2.09100	1.66510	0.01110
H	-2.07510	1.55760	0.96780
H	-2.68920	-0.10040	-0.47180
O	-0.52120	-0.90700	1.35260
O	-2.65470	-1.06860	-0.55000
H	-1.26380	-0.95310	0.72950
H	-2.15990	-1.22890	-1.36030
C	0.66800	-1.17190	0.62740
C	1.21180	0.04550	-0.11720
H	0.49640	-1.97650	-0.09540
H	1.41970	-1.51200	1.34060
C	1.47490	1.20760	0.82210
H	2.22610	0.92700	1.55970
H	1.84290	2.06540	0.25900
H	0.56340	1.49830	1.34380
C	2.46800	-0.35480	-0.87460
H	2.24590	-1.15210	-1.58610
H	2.86210	0.50170	-1.42100
H	3.23370	-0.71050	-0.18510

$HO\text{-}H_2C\text{-}COH\text{-}(CH_3)_2\cdots(H_2O)_3$

E(RM062X)=-538.210222116

O	1.36460	1.58890	0.01180
H	1.92730	1.79080	-0.74600
H	-0.31490	2.21560	-0.27500
O	-1.23650	2.52610	-0.35750
H	-1.35130	2.73140	-1.29070
H	-2.30800	1.11560	-0.03010
O	-2.93840	0.38840	0.14200
H	-3.26810	0.55170	1.03140
H	-2.19740	-1.24700	0.24410
O	0.57100	-1.84860	-1.00080
O	-1.84840	-2.15830	0.30710
H	-0.24400	-2.06690	-0.51310
H	-2.41570	-2.68140	-0.26820
C	0.66320	-0.43530	-1.04320
C	1.34000	0.15900	0.19530
H	-0.33180	0.01010	-1.14600
H	1.25110	-0.16590	-1.92380
C	0.51490	-0.08970	1.44320
H	0.43340	-1.15970	1.63170
H	0.98930	0.37800	2.30600
H	-0.48980	0.32070	1.32500
C	2.76090	-0.35450	0.34970
H	3.23220	0.10670	1.21760
H	2.76650	-1.43510	0.48500
H	3.34790	-0.11340	-0.53870

$HO\text{-}H_2C\text{-}COH\text{-}(CH_3)_2\cdots(H_2O)_4$
E(RM062X)=-614.654391409

O	2.04210	-1.21630	-0.35850
H	2.82440	-1.28460	0.20220
H	0.72030	-2.35020	0.20950
O	-0.01560	-2.90030	0.53680
H	-0.24050	-3.48230	-0.19610
H	-1.41640	-1.76720	0.75010
O	-2.21290	-1.21260	0.86430
H	-1.88660	-0.37520	1.21280
H	-2.71110	-0.49330	-0.76950
O	-2.99120	0.14230	-1.45410
H	-2.33240	0.06600	-2.15170
H	-2.31240	1.45130	-0.28630
O	0.64380	1.74660	1.29670
O	-1.99430	2.03900	0.42210
H	-0.26910	1.79020	0.96130
H	-2.60400	1.89850	1.15400
C	1.13790	0.43230	1.11130
C	1.57570	0.14700	-0.32830
H	0.38880	-0.31070	1.40300
H	2.00320	0.31590	1.76780
C	0.39620	0.20450	-1.28080
H	-0.03960	1.20370	-1.28530
H	0.71850	-0.03550	-2.29430
H	-0.36870	-0.51080	-0.97400
C	2.69490	1.07760	-0.76110
H	3.54760	0.98490	-0.08570
H	3.01800	0.82850	-1.77180
H	2.35700	2.11300	-0.74980

Hydrolysis of 2,2-dimethyloxirane at 333 K. The nucleophilic substitution reaction occurs on the least substituted carbon atom.

$H_2C\text{-}O\text{-}C\text{-}(CH_3)_2\cdots H_2O$
E(RM062X)=-308.845287409

C	0.28990	-1.04340	0.87600
C	0.80430	0.08450	0.09590
O	-2.85800	0.18710	-0.23850
H	-3.40310	-0.48900	-0.65110
O	-0.20670	-0.79120	-0.45180
H	-1.94740	-0.13920	-0.32980
C	0.32170	1.47630	0.39000
H	0.23410	2.04610	-0.53620
H	-0.64640	1.45570	0.88820
H	1.03700	1.98630	1.03530
C	2.14230	-0.02920	-0.57580
H	2.37820	-1.06990	-0.79150
H	2.14580	0.53790	-1.50750

H	2.91700	0.37980	0.07300
H	-0.43070	-0.86010	1.66360
H	0.88390	-1.94420	0.96270

H_2C-O-C-$(CH_3)_2\cdots(H_2O)_2$

E(RM062X)=-385.288618565

C	1.36450	-0.08420	0.11710
C	0.25700	-0.97010	0.48390
H	0.38450	-2.04290	0.41540
O	0.25570	-0.29220	-0.78670
H	-2.55900	-1.62330	0.28280
O	-3.24180	-0.94630	0.29010
H	-2.78730	-0.13330	0.01020
O	-1.92480	1.43280	-0.53630
H	-1.08680	0.95310	-0.66500
H	-1.78800	1.95990	0.25720
C	1.43000	1.29690	0.70340
H	2.09220	1.30030	1.56930
H	1.82730	1.99920	-0.03080
H	0.44270	1.63250	1.01870
C	2.66190	-0.66890	-0.36130
H	2.50600	-1.65500	-0.79540
H	3.11200	-0.01640	-1.11070
H	3.35740	-0.75680	0.47330
H	-0.49380	-0.61330	1.17940

H_2C-O-C-$(CH_3)_2\cdots(H_2O)_3$

E(RM062X)=-461.733487423

O	1.47020	2.51600	-0.08860
H	0.51640	2.39690	-0.10890
H	1.83710	1.61460	-0.05210
O	2.82200	0.04740	-0.03260
H	3.18370	0.02670	-0.92420
H	2.28020	-0.76210	0.03790
O	-1.12720	-1.18280	-0.57200
O	1.31190	-2.29420	0.21150
H	0.41490	-1.97750	0.00130
H	1.30510	-2.43950	1.16320
C	-1.40100	0.08370	0.06850
C	-0.67470	0.02970	-1.20430
C	-0.65180	0.30310	1.35320
H	-1.08190	-0.31480	2.14310
H	0.40390	0.05820	1.24100
H	-0.73840	1.34690	1.65700
C	-2.85450	0.46010	0.07680
H	-3.32100	0.22250	-0.87770
H	-3.37570	-0.07430	0.87230
H	-2.95760	1.52930	0.26300
H	0.40250	0.14990	-1.20570

H	-1.19270	0.27260	-2.12320

H_2C-O-C-$(CH_3)_2\cdots(H_2O)_4$

E(RM062X)=-538.178361439

O	-1.70800	2.49340	-0.65870
H	-2.19040	1.68390	-0.46720
H	-0.85460	2.39780	-0.19840
O	0.76070	2.48130	0.67460
H	0.54390	2.15530	1.55360
H	1.42810	1.85520	0.33270
O	2.78010	0.84520	-0.33920
H	2.72560	1.00030	-1.28760
H	2.60960	-0.11060	-0.23080
O	-0.36670	-1.75190	-0.68560
O	2.33260	-1.89450	-0.01670
H	1.37840	-1.92830	-0.21420
H	2.38950	-2.01410	0.93700
C	-1.11080	-0.85080	0.16480
C	-0.54250	-0.38360	-1.10310
C	-0.42820	-0.50790	1.45890
H	-0.91920	0.35330	1.91460
H	-0.50200	-1.34590	2.15390
H	0.62250	-0.26830	1.29680
C	-2.57820	-1.16000	0.25070
H	-2.75080	-1.97450	0.95520
H	-3.11840	-0.28230	0.60940
H	-2.97130	-1.44100	-0.72480
H	0.36580	0.20780	-1.08920
H	-1.18850	-0.26320	-1.96350

H_2C-O-C-$(CH_3)_2\cdots(H_2O)_5$

E(RM062X)=-614.62528145

O	-1.14740	-1.46280	-1.75100
H	-0.22380	-1.70160	-1.62400
H	-1.58730	-1.69260	-0.91000
O	-2.54810	-1.92260	0.62600
H	-3.43450	-2.17210	0.34610
H	-2.62730	-0.99510	0.91830
O	-2.67410	0.81260	1.26760
H	-1.90990	0.95720	1.83530
H	-2.36140	1.03280	0.36910
O	-1.68060	1.28550	-1.32490
H	-1.37560	0.37810	-1.50240
H	-0.92500	1.74880	-0.92290
O	2.31140	0.89660	0.08040
O	0.19050	2.71140	0.24200
H	0.95970	2.11450	0.27480
H	-0.29080	2.53440	1.05760
C	1.87710	-0.47280	0.24340

C	1.92080	0.14640	-1.08520
H	0.99940	0.49020	-1.54210
H	2.73650	-0.08910	-1.75670
C	0.56220	-0.62640	0.95520
H	0.20690	-1.65200	0.85350
H	0.68640	-0.41370	2.01860
H	-0.18700	0.04550	0.53780
C	2.97230	-1.41260	0.65810
H	3.15340	-1.32800	1.73050
H	2.67870	-2.44020	0.44340
H	3.89400	-1.19080	0.12280

$[H_2C\text{-}O\text{-}C\text{-}(CH_3)_2\cdots H_2O]^{\ddagger}$

E(RM062X)=-308.757826215

C	-0.39910	-0.44480	0.97830
C	0.58540	0.00390	-0.01240
O	-2.40460	0.11020	-0.00470
H	-2.87250	-0.73080	0.03330
O	-0.21060	-0.32610	-1.12660
H	-1.66760	-0.02130	-0.68500
C	0.88140	1.49210	0.08200
H	1.51900	1.78670	-0.75100
H	-0.04540	2.06440	0.03340
H	1.39260	1.72700	1.01640
C	1.85800	-0.83430	0.04320
H	1.61690	-1.89600	0.00870
H	2.45670	-0.57970	-0.83330
H	2.44150	-0.62520	0.93970
H	-0.85280	0.20380	1.71440
H	-0.62050	-1.50310	1.02660

$[H_2C\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_2]^{\ddagger}$

E(RM062X)=-385.203634022

C	0.96290	0.02740	0.00230
C	0.37720	-1.22920	0.47880
H	0.44810	-2.09700	-0.16280
O	0.03960	0.23420	-1.03620
H	-1.92210	-1.77990	-0.58840
O	-1.87950	-1.40350	0.29790
H	-2.13160	-0.46780	0.17480
O	-2.16410	1.30250	-0.34320
H	-1.23760	0.96440	-0.60100
H	-2.02950	1.88870	0.40650
C	0.94010	1.12740	1.05370
H	1.62470	0.89510	1.87040
H	1.24690	2.06820	0.59680
H	-0.06300	1.24630	1.46450
C	2.37480	-0.20450	-0.53120
H	2.37060	-1.00190	-1.27340

H	2.70180	0.72100	-1.00900
H	3.07550	-0.45590	0.26530
H	0.01890	-1.37350	1.48740

$[H_2C\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_3]^{\ddagger}$

E(RM062X)=-461.681428095

O	0.14870	2.15460	-0.50210
H	-0.47060	2.46090	0.17420
H	0.98330	1.93660	-0.03500
O	2.45290	0.90460	0.46350
H	3.23730	1.18220	-0.02110
H	2.31350	-0.02450	0.21000
O	-0.90350	-1.43830	-0.65260
O	1.76450	-1.86920	-0.36610
H	0.77770	-1.81300	-0.44660
H	1.92140	-2.35740	0.44780
C	-1.09080	-0.26640	0.11150
C	-0.34140	0.38620	-0.97010
C	-0.45650	-0.29700	1.49050
H	-1.00580	-1.00540	2.11310
H	0.58450	-0.60870	1.45220
H	-0.51380	0.68420	1.96470
C	-2.54430	0.16610	0.18900
H	-2.99420	0.16000	-0.80360
H	-3.09920	-0.52110	0.82920
H	-2.63090	1.17030	0.60870
H	0.69510	0.13530	-1.10610
H	-0.90020	0.65330	-1.85500

$[H_2C\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_4]^{\ddagger}$

E(RM062X)=-538.133331946

O	-0.47500	2.11650	-0.92000
H	-1.24730	2.43450	-0.43550
H	0.30140	2.20480	-0.30450
O	1.69920	2.12150	0.59040
H	1.41010	2.02430	1.50390
H	2.07050	1.24630	0.34770
O	2.83940	-0.26570	-0.16790
H	3.09790	-0.13900	-1.08620
H	2.25430	-1.05490	-0.17150
O	-1.11750	-1.55700	-0.49190
O	1.25240	-2.49930	-0.15140
H	0.31150	-2.13700	-0.25070
H	1.31020	-2.80930	0.75740
C	-1.31350	-0.31820	0.16020
C	-0.66040	0.21430	-1.03690
C	-0.54290	-0.17260	1.45840
H	-0.64870	0.83780	1.85770
H	-0.94100	-0.87500	2.19280

H	0.51670	-0.38130	1.31040
C	-2.77680	0.04180	0.31650
H	-3.23560	-0.61600	1.05610
H	-2.89160	1.07230	0.65750
H	-3.29970	-0.07710	-0.63230
H	0.40850	0.08100	-1.12400
H	-1.24450	0.26790	-1.94160

$[H_2C\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_5]^{\ddagger}$

E(RM062X)=-614.576364964

O	0.66670	-2.01640	-1.2314
H	1.23460	-2.57800	-0.6884
H	-0.22640	-2.02910	-0.8017
O	-1.79470	-2.10130	-0.2168
H	-2.41480	-2.13210	-0.9531
H	-2.16160	-1.43910	0.3987
O	-3.01620	-0.11780	1.3805
H	-2.41530	0.10120	2.0999
H	-2.77460	0.48800	0.6555
O	-2.24170	1.10130	-1.0177
H	-1.89250	0.23650	-1.2603
H	-1.45430	1.66790	-0.8711
O	1.92680	1.32770	-0.1003
O	-0.13870	2.81820	-0.5205
H	0.66520	2.23800	-0.3200
H	-0.41410	3.16860	0.3320
C	1.59560	0.04580	0.3962
C	1.30890	-0.23180	-1.0114
H	0.40500	0.18520	-1.4305
H	2.14600	-0.39200	-1.6722
C	0.39750	0.03000	1.3244
H	0.10680	-0.99500	1.5624
H	0.65060	0.54130	2.2547
H	-0.44910	0.53850	0.8644
C	2.78590	-0.69100	0.9749
H	3.08800	-0.21600	1.9094
H	2.53620	-1.73260	1.1849
H	3.62500	-0.66260	0.2800

$HO\text{-}H_2C\text{-}COH\text{-}(CH_3)_2$

E(RM062X)=-308.875472556

C	0.84440	-0.70620	-0.45400
C	-0.41340	0.00370	0.02430
O	1.97870	0.04860	-0.03440
H	2.76310	-0.49510	-0.14860
O	-0.38450	0.07790	1.45770
H	0.43590	0.52060	1.70510
C	-0.50850	1.40790	-0.55780
H	-1.42440	1.88780	-0.21340

H	0.34060	2.01490	-0.24380
H	-0.52270	1.36960	-1.64730
C	-1.62970	-0.82560	-0.34180
H	-1.55880	-1.82300	0.09290
H	-2.53400	-0.34400	0.02970
H	-1.71000	-0.92140	-1.42430
H	0.82240	-0.79350	-1.54300
H	0.87670	-1.70710	-0.01810

$HO\text{-}H_2C\text{-}COH\text{-}(CH_3)_2\cdots(H_2O)$

E(RM062X)=-385.32011131

C	-0.81410	-0.15550	-0.01440
C	-0.41040	1.30430	-0.17170
H	-0.57300	1.60470	-1.20860
O	-0.13930	-0.95620	-0.99450
H	1.24760	2.34590	-0.11250
O	0.96560	1.47270	0.17560
H	2.24520	0.12110	0.00240
O	2.66650	-0.72590	-0.22060
H	0.80180	-0.99860	-0.76590
H	2.73150	-1.19510	0.61720
C	-0.49550	-0.67050	1.38340
H	-0.97620	-0.04860	2.13900
H	-0.85950	-1.69240	1.49040
H	0.57980	-0.66390	1.56350
C	-2.29780	-0.27650	-0.31640
H	-2.51800	0.11010	-1.31210
H	-2.59710	-1.32330	-0.27400
H	-2.88430	0.28180	0.41230
H	-1.03340	1.92250	0.47860

$HO\text{-}H_2C\text{-}COH\text{-}(CH_3)_2\cdots(H_2O)_2$

E(RM062X)=-461.76502773

O	-0.54620	-1.04830	1.18700
H	-0.45650	-0.42370	1.91460
H	-1.93230	-1.09780	0.00550
O	-2.67770	-1.01810	-0.61670
H	-2.26330	-0.98560	-1.48500
H	-2.52160	0.84000	-0.17740
O	0.26260	0.46970	-1.13390
O	-2.09650	1.68390	0.04980
H	-0.50280	0.86690	-0.68730
H	-1.84950	1.58580	0.97550
C	1.21070	0.06180	-0.14180
C	0.71440	-1.21040	0.54070
C	1.41940	1.18450	0.86670
H	1.78610	2.07500	0.35660
H	0.48480	1.44390	1.36910
H	2.14800	0.88860	1.62180

C	2.50160	-0.25880	-0.87470
H	2.33220	-1.03370	-1.62320
H	2.87690	0.63400	-1.37430
H	3.25990	-0.61020	-0.17550
H	0.56350	-1.98210	-0.21400
H	1.46060	-1.56010	1.25740

$HO\text{-}H_2C\text{-}COH\text{-}(CH_3)_2\cdots(H_2O)_3$

E(RM062X)=-538.209708449

O	0.43550	-1.81900	-0.94320
H	1.29100	-2.25800	-0.89290
H	-0.99080	-2.11940	0.13680
O	-1.85570	-2.14280	0.58520
H	-1.65370	-2.00120	1.51570
H	-2.52620	-0.53580	0.06540
O	-2.91660	0.31900	-0.20120
H	-3.15180	0.20790	-1.12780
H	-1.80070	1.74190	-0.15510
O	1.39740	1.63220	-0.15300
O	-1.25780	2.55420	-0.16140
H	0.48390	1.97410	-0.15610
H	-1.38490	2.94290	0.70990
C	1.33830	0.22910	0.11860
C	0.62930	-0.41340	-1.07650
C	0.57690	-0.02300	1.41290
H	0.56000	-1.08650	1.65190
H	1.06320	0.50670	2.23260
H	-0.45290	0.33070	1.32790
C	2.77420	-0.25320	0.22420
H	3.27320	0.24280	1.05690
H	2.81290	-1.32860	0.40070
H	3.31720	-0.02950	-0.69480
H	-0.36850	0.01900	-1.17230
H	1.19400	-0.19340	-1.98540

$HO\text{-}H_2C\text{-}COH\text{-}(CH_3)_2\cdots(H_2O)_4$

E(RM062X)=-614.653256727

O	0.47600	-1.67060	-1.25860
H	1.07870	-2.40000	-1.07940
H	-1.20050	-1.86120	-0.57180
O	-2.10370	-2.03020	-0.24610
H	-2.67930	-1.82480	-0.99020
H	-2.62150	-0.77630	0.97650
O	-2.98150	0.00450	1.43900
H	-2.32370	0.22560	2.10560
H	-2.43250	0.92220	-0.12760
O	-2.11300	1.20970	-1.00090
H	-1.77420	0.40180	-1.40260
H	-0.66210	2.30150	-0.64770

O	2.19860	1.17860	0.28030
O	0.08130	2.91000	-0.47690
H	1.50400	1.81520	0.03080
H	-0.15430	3.36190	0.33960
C	1.59970	-0.12120	0.31530
C	1.17940	-0.43950	-1.12230
H	0.50260	0.33940	-1.47570
H	2.06670	-0.44010	-1.75940
C	0.40180	-0.11730	1.25490
H	-0.05110	-1.10690	1.31720
H	0.72180	0.17870	2.25450
H	-0.35160	0.59000	0.90510
C	2.67000	-1.08390	0.79660
H	2.98780	-0.81380	1.80390
H	2.28660	-2.10430	0.82610
H	3.53600	-1.05350	0.13430

Hydrolysis of cis 2,3-dimethyloxirane at 333 K.

H_3C-CH-O-CH-CH_3···H_2O
E(RM062X)=-308.844022888

C	-0.37470	-0.74660	0.34030
H	0.31950	-1.28490	0.97730
C	-0.23660	0.71420	0.32590
O	3.00310	-0.13500	0.00840
H	2.94540	0.37210	0.82350
O	0.29370	-0.08380	-0.75390
H	2.09670	-0.13520	-0.34260
H	0.54790	1.12390	0.95450
C	-1.64120	-1.47580	0.01770
H	-1.41220	-2.42920	-0.45810
H	-2.18510	-1.68220	0.93980
H	-2.28110	-0.90050	-0.64650
C	-1.34060	1.66480	-0.01670
H	-1.85730	1.96770	0.89440
H	-0.92870	2.55960	-0.48320
H	-2.06130	1.21970	-0.69820

H_3C-CH-O-CH-CH_3···$(H_2O)_2$
E(RM062X)=-385.287338524

C	0.43390	0.49870	-0.43350
H	-0.38570	0.39450	-1.13780
C	1.31800	-0.66480	-0.30150
H	1.06920	-1.52220	-0.91820
O	0.30270	-0.39890	0.69060
H	-2.13630	1.42820	0.51300
O	-2.90300	0.99190	0.12950
H	-2.63010	0.06530	0.02350
O	-2.01710	-1.71740	-0.08050

H	-1.16110	-1.39000	0.25110
H	-1.86670	-1.89820	-1.01380
C	2.74220	-0.59600	0.15230
H	2.99770	-1.49330	0.71580
H	3.39710	-0.54840	-0.71820
H	2.92770	0.27270	0.77910
C	0.83190	1.90780	-0.12480
H	1.20120	2.38960	-1.03040
H	-0.03450	2.47050	0.22550
H	1.60470	1.95190	0.63860

H_3C-CH-O-CH-$CH_3\cdots(H_2O)_3$

E(RM062X)=-461.73226942

O	0.43160	2.71980	-0.04370
H	-0.41730	2.32540	0.17670
H	1.07940	1.99760	0.03870
O	2.51800	0.82990	0.18480
H	3.11360	1.07420	-0.53040
H	2.31970	-0.11390	0.03820
O	-0.75820	-1.52890	-0.04400
O	2.01280	-1.92000	-0.17780
H	1.04570	-1.99210	-0.10130
H	2.35970	-2.33890	0.61610
C	-0.68820	-0.31830	0.73860
C	-0.68710	-0.25960	-0.72870
C	-1.86960	0.13920	-1.55500
H	-1.85870	-0.39610	-2.50430
H	-2.80830	-0.06980	-1.04830
H	-1.81500	1.20730	-1.76980
C	-1.87340	0.01720	1.58910
H	-1.85280	-0.56760	2.50850
H	-1.83470	1.07340	1.86070
H	-2.81010	-0.17860	1.07350
H	0.27870	-0.10050	-1.19850
H	0.27630	-0.19700	1.22190

H_3C-CH-O-CH-$CH_3\cdots(H_2O)_4$

E(RM062X)=-538.177707005

O	-1.34180	-1.64340	-1.38170
H	-0.45300	-1.96970	-1.20860
H	-1.75930	-1.57900	-0.50670
O	-2.73020	-0.80480	0.97190
H	-2.13370	-0.84220	1.72680
H	-2.53110	0.03970	0.53320
O	-1.93950	1.21370	-0.90990
H	-1.51060	0.42070	-1.26300
H	-1.21520	1.77520	-0.58140
O	1.77790	0.71650	0.66750
O	0.10520	2.92600	0.10250

H	0.78740	2.31650	0.43080
H	-0.27810	3.32130	0.89180
C	0.67290	-0.21030	0.73900
C	1.34840	0.04620	-0.53740
H	0.83830	0.71610	-1.22360
H	-0.27160	0.30050	0.89020
C	2.32420	-0.89350	-1.17450
H	1.79930	-1.54250	-1.87730
H	3.07230	-0.33160	-1.73350
H	2.83220	-1.51050	-0.43760
C	0.85400	-1.45350	1.55200
H	0.70910	-1.23580	2.61020
H	0.10250	-2.18720	1.25340
H	1.84120	-1.88910	1.41750

H_3C-CH-O-CH-$CH_3 \cdots (H_2O)_5$

E(RM062X)=-614.624139782

O	-0.56240	-1.62690	-1.72650
H	0.36260	-1.79590	-1.51920
H	-1.04730	-1.82050	-0.90100
O	-2.12090	-1.98480	0.56900
H	-2.91590	-2.42960	0.25810
H	-2.39050	-1.05820	0.71450
O	-2.79750	0.72170	0.79550
H	-2.19220	1.10980	1.43610
H	-2.38290	0.89720	-0.07090
O	-1.41500	1.10550	-1.61380
H	-0.97530	0.23860	-1.65230
H	-0.82400	1.68680	-1.10410
O	1.71760	0.87820	0.95560
O	-0.08470	2.86660	0.17820
H	0.58040	2.29260	0.59680
H	-0.79210	2.94320	0.82700
C	0.84110	-0.23640	0.68000
C	1.75970	0.25990	-0.34930
H	1.32400	0.89060	-1.11810
H	-0.19730	0.06870	0.58180
C	3.02690	-0.43350	-0.74160
H	2.81790	-1.13020	-1.55520
H	3.75720	0.29170	-1.10000
H	3.46160	-0.98420	0.08870
C	1.06820	-1.49500	1.45900
H	0.56920	-1.43470	2.42610
H	0.64480	-2.34000	0.91410
H	2.12690	-1.67860	1.62450

$[H_3C$-CH-O-CH-$CH_3 \cdots H_2O]^{\ddagger}$

E(RM062X)=-308.771060139

C	-0.09900	0.66980	0.57730

H	-0.64960	0.82040	1.49940
C	0.67290	-0.58290	0.36940
O	-2.32710	-0.41640	0.03480
H	-2.55760	-0.91250	0.82620
O	-0.02920	-1.15740	-0.69740
H	-1.48570	-0.86170	-0.33030
H	0.61590	-1.18950	1.27930
C	-0.10660	1.75440	-0.37240
H	-1.06990	2.25770	-0.42430
H	0.56920	2.47760	0.12710
H	0.30160	1.50460	-1.34520
C	2.13810	-0.30060	0.05250
H	2.64220	0.20120	0.87890
H	2.62610	-1.25900	-0.12410
H	2.22590	0.30760	-0.84690

$[H_3C\text{-}CH\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_2]^{\ddagger}$

E(RM062X)=-385.216893731

C	0.68550	0.77030	-0.53100
H	0.25450	1.17450	-1.43860
C	0.73190	-0.69440	-0.32100
H	0.26090	-1.18870	-1.17890
O	-0.02660	-0.83560	0.84370
H	-1.70160	1.73130	0.65740
O	-1.84400	1.46610	-0.25680
H	-2.15330	0.54180	-0.19840
O	-2.37750	-1.24860	0.06300
H	-1.40450	-1.13440	0.39510
H	-2.31390	-1.71030	-0.77760
C	2.16950	-1.19090	-0.19000
H	2.13040	-2.26330	0.00070
H	2.74170	-1.01660	-1.10180
H	2.66670	-0.70180	0.64700
C	1.26400	1.71230	0.39480
H	2.17830	2.01530	-0.15400
H	0.67590	2.62460	0.48100
H	1.54390	1.28860	1.35230

$[H_3C\text{-}CH\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_3]^{\ddagger}$

E(RM062X)=-461.683776816

O	-0.22130	2.08680	0.09140
H	-0.71280	2.15390	0.91990
H	0.71200	1.90390	0.34350
O	2.32870	1.18430	0.51710
H	2.96490	1.66210	-0.02410
H	2.30640	0.27780	0.14700
O	-0.38880	-1.70700	-0.30070
O	2.18940	-1.42710	-0.52990
H	1.20680	-1.63930	-0.46840

H	2.61610	-1.98360	0.12800
C	-0.54170	-0.61790	0.57990
C	-0.57230	0.23940	-0.61160
C	-1.82910	0.52330	-1.35450
H	-1.64190	1.22650	-2.16130
H	-2.20580	-0.40310	-1.78630
H	-2.59010	0.92390	-0.68690
C	-1.78310	-0.65760	1.44030
H	-1.66990	-1.42600	2.20480
H	-1.93700	0.30140	1.93930
H	-2.66450	-0.89180	0.84410
H	0.36370	0.31610	-1.14370
H	0.34540	-0.44050	1.19730

$[H_3C\text{-}CH\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_4]^{\ddagger}$

E(RM062X)=-538.129907668

O	-0.63940	1.86320	-0.83540
H	-1.44720	2.21620	-0.44130
H	0.08350	2.07830	-0.19650
O	1.45210	2.27160	0.81500
H	1.16790	1.97040	1.68420
H	1.92440	1.50950	0.41900
O	2.64270	0.24190	-0.60330
H	2.31330	0.45750	-1.48170
H	2.30680	-0.66410	-0.42010
O	-0.69790	-1.79190	0.32010
O	1.75710	-2.29660	-0.11110
H	0.76570	-2.14860	0.08170
H	2.15090	-2.55710	0.72650
C	-0.65080	-0.43950	0.71500
C	-0.84360	-0.12300	-0.70470
H	0.03420	-0.26220	-1.32050
H	0.34200	-0.14510	1.07110
C	-2.17570	-0.16980	-1.37340
H	-2.10890	0.30350	-2.34990
H	-2.47190	-1.20610	-1.52110
H	-2.93770	0.33030	-0.77850
C	-1.71500	-0.01220	1.69570
H	-1.51320	-0.46280	2.66740
H	-1.71280	1.07320	1.81430
H	-2.70330	-0.33170	1.36740

$[H_3C\text{-}CH\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_5]^{\ddagger}$

E(RM062X)=-614.573821073

O	-0.83180	1.57030	-1.29600
H	-1.55090	2.17810	-1.08200
H	-0.06940	1.86220	-0.73670
O	1.20960	2.40470	0.24810
H	1.75440	3.02770	-0.24390

H	1.81920	1.69440	0.52540
O	2.96690	0.30570	0.87430
H	2.53810	-0.23970	1.54190
H	2.69380	-0.08300	0.02050
O	1.96890	-0.56260	-1.57680
H	1.31450	0.13480	-1.69100
H	1.48920	-1.31330	-1.16350
O	-1.14070	-1.60080	0.82050
O	0.90800	-2.70070	-0.22290
H	0.07710	-2.31390	0.22360
H	1.58100	-2.72040	0.46460
C	-0.75090	-0.24670	0.77380
C	-1.37820	-0.20580	-0.55060
H	-0.82280	-0.70630	-1.33070
H	0.33660	-0.12400	0.71300
C	-2.84430	-0.04040	-0.75620
H	-3.03360	0.25280	-1.78650
H	-3.34170	-0.99400	-0.58860
H	-3.26500	0.70160	-0.08040
C	-1.32390	0.62440	1.86580
H	-0.82990	0.39310	2.80940
H	-1.16100	1.68050	1.64440
H	-2.39220	0.44790	1.98580

H_3C-CHOH-CHOH-CH_3

E(RM062X)=-308.875676476

C	-0.67500	0.27360	0.45240
H	-0.72610	0.74230	1.43910
C	0.69910	-0.38100	0.32110
O	-1.68170	-0.74160	0.35660
H	-1.55400	-1.36200	1.08270
O	0.80010	-1.09410	-0.91160
H	-0.00190	-1.62220	-1.00200
H	0.79170	-1.09410	1.14860
C	-0.97920	1.29920	-0.61810
H	-1.99530	1.67110	-0.49490
H	-0.29740	2.14470	-0.54450
H	-0.88680	0.86020	-1.61160
C	1.84280	0.60640	0.38200
H	1.77220	1.21390	1.28430
H	2.79430	0.07670	0.39850
H	1.82970	1.26560	-0.48580

H_3C-CHOH-CHOH-$CH_3\cdots(H_2O)$

E(RM062X)=-385.31916592

C	0.56730	0.83040	-0.41900
H	1.15830	1.11690	-1.29330
C	0.56240	-0.69500	-0.36130
H	0.03720	-1.04520	-1.25590

O	-0.11510	-1.18370	0.79440
H	-0.85040	2.19260	-0.51860
O	-0.79270	1.23900	-0.63760
H	-2.29700	0.22200	-0.21770
O	-2.83510	-0.48500	0.17580
H	-1.06620	-1.03790	0.67690
H	-3.12120	-1.02640	-0.56630
C	1.96560	-1.26430	-0.34670
H	1.92670	-2.35020	-0.41750
H	2.54450	-0.88280	-1.18710
H	2.47720	-0.99760	0.57840
C	1.12680	1.49910	0.82020
H	2.17760	1.24720	0.95700
H	1.05260	2.58260	0.71800
H	0.57120	1.19430	1.70630

H_3C-CHOH-CHOH-$CH_3\cdots(H_2O)_2$

E(RM062X)=-461.76389362

O	-0.37300	1.80790	0.13260
H	-1.11250	1.99320	0.72280
H	1.43200	1.59650	0.56930
O	2.34110	1.26120	0.64980
H	2.88230	1.87140	0.13910
H	2.36550	-0.36970	-0.20920
O	-0.32760	-1.82720	-0.17450
O	2.38170	-1.23020	-0.66920
H	0.59520	-1.80320	-0.48050
H	2.88860	-1.81050	-0.09280
C	-0.54700	-0.59330	0.50460
C	-0.59740	0.55080	-0.51860
C	-1.86630	0.58910	-1.34520
H	-1.77320	1.33000	-2.13800
H	-2.05530	-0.38370	-1.79930
H	-2.72240	0.85400	-0.72310
C	-1.80410	-0.73070	1.33700
H	-1.65470	-1.47700	2.11610
H	-2.05910	0.21510	1.81700
H	-2.64430	-1.04170	0.71600
H	0.26520	0.42600	-1.17650
H	0.30360	-0.39030	1.16360

H_3C-CHOH-CHOH-$CH_3\cdots(H_2O)_3$

E(RM062X)=-538.207960657

O	-0.39500	1.60250	-0.76380
H	-1.17860	2.12230	-0.54880
H	0.89270	2.02600	0.45740
O	1.71190	2.14240	0.97440
H	1.51550	1.76540	1.83790
H	2.44640	0.78460	-0.02670

O	2.75900	0.09510	-0.64120
H	2.35890	0.32300	-1.48690
H	2.03590	-1.50170	-0.22500
O	-0.95680	-1.72580	0.66290
O	1.65540	-2.38420	-0.04600
H	-0.07840	-2.05750	0.40140
H	2.10700	-2.69740	0.74380
C	-0.87970	-0.30390	0.66750
C	-0.75650	0.21390	-0.77180
H	0.09590	-0.29670	-1.22510
H	0.03030	0.00490	1.19420
C	-1.99400	-0.00760	-1.61760
H	-1.79180	0.25870	-2.65410
H	-2.30160	-1.05210	-1.58120
H	-2.81940	0.60890	-1.25720
C	-2.09060	0.22900	1.40480
H	-2.05280	-0.07460	2.45020
H	-2.12260	1.31860	1.36790
H	-3.00850	-0.16160	0.96500

H_3C-CHOH-CHOH-$CH_3\cdots(H_2O)_4$

E(RM062X)=-614.65368088

O	0.69490	-1.06210	-1.34460
H	1.26270	-1.83250	-1.22590
H	-0.67880	-1.98200	-0.25150
O	-1.33320	-2.40410	0.32750
H	-1.90490	-2.90200	-0.26620
H	-2.38880	-0.96840	0.82630
O	-2.95350	-0.17400	0.85930
H	-2.44710	0.47250	1.36250
H	-2.30870	0.17760	-0.87830
O	-1.81090	0.41760	-1.67910
H	-1.08400	-0.21880	-1.71400
H	-1.17480	1.90880	-0.71490
O	1.15170	1.43920	1.27580
O	-0.97280	2.65850	-0.12630
H	0.52800	2.05700	0.85830
H	-1.69400	2.66270	0.51160
C	0.84420	0.15490	0.74150
C	1.31550	0.07170	-0.71440
H	0.91340	0.94520	-1.23240
H	-0.24420	0.03130	0.72220
C	2.81870	0.02510	-0.88430
H	3.08090	0.09130	-1.93930
H	3.28700	0.85580	-0.35750
H	3.22080	-0.90770	-0.48460
C	1.45500	-0.90070	1.63840
H	0.96060	-0.90060	2.60900
H	1.34450	-1.89190	1.19660

H	2.51670	-0.70480	1.79080

Hydrolysis of trans 2,3-dimethyloxirane at 333 K.

H_3C-CH-O-CH-$CH_3 \cdots H_2O$

E(RM062X)=-308.846108828

C	-0.89260	0.26820	-0.37280
H	-0.36610	0.55740	-1.27700
C	-0.42160	-0.94650	0.29500
H	-1.13120	-1.45360	0.93970
O	2.50750	1.21590	-0.05820
H	2.67750	0.73130	-0.87110
O	-0.05740	0.35540	0.80020
H	1.64230	0.89280	0.24360
C	-2.28900	0.77970	-0.21680
H	-2.29930	1.86970	-0.21410
H	-2.90470	0.43750	-1.04860
H	-2.72370	0.41930	0.71460
C	0.69820	-1.77640	-0.24920
H	1.32510	-2.15060	0.56040
H	0.29380	-2.63270	-0.78870
H	1.31430	-1.19110	-0.93120

H_3C-CH-O-CH-$CH_3 \cdots (H_2O)_2$

E(RM062X)=-385.289606266

C	1.64360	0.01720	-0.19360
C	0.52740	-0.78900	0.30320
O	0.38920	-0.01360	-0.90730
H	-2.32450	-1.11560	-0.29730
O	-2.87520	-0.51190	0.21030
H	-2.43080	0.34830	0.13000
O	-1.44600	1.94010	-0.12680
H	-0.71990	1.37490	-0.44700
H	-1.15950	2.23350	0.74390
C	2.01640	1.32960	0.42100
H	1.17040	1.75490	0.96100
H	2.84150	1.18860	1.11900
H	2.33770	2.03490	-0.34570
C	0.47380	-2.27450	0.13820
H	0.86700	-2.75900	1.03190
H	-0.55330	-2.61250	-0.00420
H	1.06970	-2.58290	-0.72000
H	-0.04110	-0.36910	1.12760
H	2.42990	-0.51200	-0.72080

H_3C-CH-O-CH-$CH_3 \cdots (H_2O)_3$

E(RM062X)=-461.734092731

O	1.29850	2.48270	0.20270
H	0.41270	2.31150	0.53530

H	1.65070	1.60950	-0.04590
O	2.57710	0.10930	-0.61500
H	2.76760	0.26430	-1.54550
H	2.05420	-0.71480	-0.59560
O	-1.38440	-1.14680	0.01200
O	1.13320	-2.28920	-0.48300
H	0.23490	-1.99400	-0.25120
H	1.48000	-2.68190	0.32460
C	-1.27990	-0.05630	0.95240
C	-1.12320	0.18270	-0.48500
H	-0.10660	0.29060	-0.85210
H	-2.24050	0.20410	1.38350
C	-2.20290	0.79800	-1.31670
H	-2.02530	1.86940	-1.41340
H	-2.21230	0.36380	-2.31640
H	-3.17640	0.64350	-0.85290
C	-0.11860	-0.10450	1.89570
H	-0.02480	0.85170	2.41150
H	-0.27000	-0.87990	2.64720
H	0.80850	-0.30440	1.35930

H_3C-CH-O-CH-$CH_3 \cdots (H_2O)_4$

E(RM062X)=-538.178438065

O	-2.97830	0.90030	0.08740
H	-2.80370	-0.00190	0.37010
H	-2.10880	1.33800	0.06500
O	-0.69520	2.53450	0.04690
H	-0.54480	2.59770	0.99560
H	0.15710	2.22980	-0.31910
O	1.76370	1.84460	-1.08790
H	1.51330	1.54750	-1.96850
H	2.18010	1.06640	-0.67030
O	0.61100	-1.85770	0.15170
O	2.97770	-0.37200	0.12150
H	2.19570	-0.95060	0.18310
H	3.12620	-0.06750	1.02270
C	-0.42070	-1.18690	0.90460
C	-0.35080	-1.04340	-0.55260
C	-1.26660	-1.78080	-1.47780
H	-1.65940	-2.67400	-0.99340
H	-2.10020	-1.14010	-1.76500
H	-0.73570	-2.07360	-2.38380
C	0.03720	-0.11300	1.84230
H	-0.81910	0.47980	2.16720
H	0.50200	-0.55240	2.72550
H	0.75380	0.54640	1.35270
H	0.08150	-0.11980	-0.92640
H	-1.16350	-1.87830	1.28910

$H_3C\text{-}CH\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_5$

E(RM062X)=-614.622667082

O	3.01400	-1.31620	0.44920
H	2.73610	-1.03790	1.32650
H	2.18640	-1.51860	-0.02290
O	0.75790	-2.09890	-1.01580
H	0.42120	-1.44850	-1.64060
H	-0.00210	-2.32390	-0.44740
O	-1.51840	-2.73350	0.51500
H	-1.32550	-2.43420	1.40880
H	-1.95350	-1.97400	0.08090
O	-2.52950	-0.68430	-1.04220
H	-1.87490	-0.71260	-1.74770
H	-2.47450	0.21860	-0.67300
O	0.25270	2.21610	0.39340
O	-2.51930	1.88810	0.05470
H	-1.58580	2.07750	0.25700
H	-2.93130	1.74160	0.91250
C	0.83860	1.01050	0.93090
C	0.69220	1.18160	-0.51400
H	1.82790	1.18610	1.34020
C	-0.06260	0.11970	1.72750
H	0.41630	-0.85250	1.86250
H	-0.25090	0.54560	2.71350
H	-1.01330	-0.02620	1.21410
C	1.84740	1.51340	-1.40290
H	2.24560	0.59530	-1.83740
H	1.53450	2.16760	-2.21650
H	2.63780	2.00290	-0.83500
H	-0.14720	0.67200	-0.97790

$[H_3C\text{-}CH\text{-}O\text{-}CH\text{-}CH_3\cdots H_2O]^{\ddagger}$

E(RM062X)=-308.771716786

C	-0.48130	-0.60070	-0.51060
H	-0.48610	-0.24270	-1.53470
C	0.76900	-0.55760	0.28980
H	0.88660	-1.55420	0.74270
O	-0.95430	1.84460	-0.26540
H	-0.36460	2.26550	-0.89860
O	0.44050	0.41250	1.24900
H	-0.34250	1.41870	0.43720
C	-1.69490	-1.18750	-0.00240
H	-2.58900	-0.65360	-0.31940
H	-1.71890	-2.14410	-0.56050
H	-1.66920	-1.39790	1.06150
C	1.99140	-0.21530	-0.53900
H	2.87030	-0.17530	0.10320
H	2.16010	-0.96490	-1.31400
H	1.85830	0.75910	-1.01240

$[H_3C\text{-}CH\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_2]^{\ddagger}$

E(RM062X)=-385.216374613

C	0.42560	-1.14080	0.18890
C	1.26960	-0.07130	-0.39320
O	-0.27480	-0.45300	1.18560
H	0.03770	2.41680	0.03120
O	-0.29370	1.95010	-0.74290
H	-1.12370	1.53660	-0.44000
O	-2.44120	0.55770	0.40020
H	-1.57820	0.08300	0.70990
H	-2.85640	-0.04460	-0.22360
C	2.32470	0.56240	0.35560
H	3.21740	0.08330	-0.09330
H	2.43070	1.62180	0.12730
H	2.30220	0.34860	1.41850
C	-0.45510	-1.82210	-0.84450
H	-1.09000	-2.55950	-0.35520
H	-1.08880	-1.08920	-1.34620
H	0.15470	-2.32830	-1.59400
H	1.12330	-1.88060	0.61700
H	1.16020	0.20490	-1.43550

$[H_3C\text{-}CH\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_3]^{\ddagger}$

E(RM062X)=-461.681182145

O	-0.75360	1.93760	0.33360
H	-1.00420	1.92220	1.26580
H	0.22600	1.98380	0.31230
O	1.96900	1.62860	-0.14540
H	2.22210	2.17760	-0.89480
H	2.03360	0.71000	-0.46800
O	-0.44550	-1.84170	-0.22390
O	1.99490	-1.12440	-1.01020
H	1.10820	-1.46830	-0.70250
H	2.63510	-1.49580	-0.39520
C	-0.75820	-0.85960	0.73570
C	-0.91360	0.08460	-0.38240
H	-0.02120	0.29310	-0.94890
H	-1.72370	-1.04770	1.21870
C	-2.22930	0.22990	-1.05970
H	-2.19870	1.01740	-1.80740
H	-2.46940	-0.70880	-1.55830
H	-3.01010	0.43630	-0.32920
C	0.30080	-0.61070	1.78820
H	0.00050	0.19070	2.46490
H	0.42480	-1.52070	2.37690
H	1.26010	-0.35480	1.34210

$[H_3C\text{-}CH\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_4]^{\ddagger}$

E(RM062X)=-538.130864521

O	1.05540	-2.00520	-0.15130
H	1.55440	-2.14150	0.66370
H	0.10560	-2.16060	0.08390
O	-1.56290	-2.28790	0.33300
H	-1.67380	-2.11380	1.27360
H	-1.90260	-1.48390	-0.11380
O	-2.51130	-0.10150	-1.04650
H	-2.19330	-0.25000	-1.94280
H	-2.12260	0.75950	-0.77490
O	0.97870	1.80980	0.22640
O	-1.48510	2.31440	-0.27300
H	-0.51530	2.11380	-0.04370
H	-1.91490	2.47960	0.57170
C	1.14290	0.57210	0.88070
C	1.10590	-0.02830	-0.45500
C	2.30210	-0.03610	-1.34280
H	3.20170	-0.26340	-0.77280
H	2.17450	-0.76810	-2.13570
H	2.41530	0.94290	-1.80430
C	0.03800	0.20580	1.84500
H	0.19820	-0.78980	2.26210
H	0.02310	0.92400	2.66580
H	-0.93120	0.22580	1.34460
H	0.12270	-0.06800	-0.90800
H	2.12580	0.47640	1.35300

$[H_3C\text{-}CH\text{-}O\text{-}CH\text{-}CH_3\cdots(H_2O)_5]^{\ddagger}$

E(RM062X)=-614.573136605

O	1.31980	-2.09540	-0.32440
H	1.47860	-2.40990	0.57420
H	0.33980	-2.10850	-0.45240
O	-1.29070	-2.00300	-0.95050
H	-1.28920	-1.27010	-1.57660
H	-1.89440	-1.71700	-0.23940
O	-3.15880	-0.98280	0.90400
H	-2.70700	-0.86230	1.74520
H	-3.02590	-0.14360	0.42090
O	-2.75070	1.14570	-0.82240
H	-2.70630	0.64720	-1.64440
H	-1.89180	1.61720	-0.76070
O	1.58860	1.61740	0.59010
O	-0.41910	2.57280	-0.71040
H	0.34870	2.19450	-0.16720
H	-0.65980	3.39950	-0.28240
C	1.36640	0.30930	1.06430
C	1.73410	-0.14180	-0.28050
H	2.09920	0.00680	1.81940
C	-0.04520	0.02900	1.52240

H	-0.16540	-1.01840	1.80460
H	-0.27960	0.64940	2.38850
H	-0.75150	0.26200	0.72490
C	3.15670	-0.27050	-0.70170
H	3.22650	-0.86030	-1.61170
H	3.56190	0.71800	-0.90880
H	3.74840	-0.73420	0.08620
H	0.98230	0.03480	-1.03960

H_3C-CHOH-CHOH-CH_3

E(RM062X)=-308.875434473

C	-0.66120	0.37170	-0.38800
H	-0.66140	1.00340	-1.28050
C	0.65130	-0.41210	-0.37460
H	0.64730	-1.07660	-1.23970
O	-0.76180	1.19510	0.77890
H	-0.09990	1.89190	0.72570
O	0.71700	-1.26510	0.76860
H	0.59800	-0.70760	1.54680
C	-1.87780	-0.52740	-0.39900
H	-2.78730	0.06960	-0.45180
H	-1.84900	-1.19220	-1.26170
H	-1.91270	-1.13330	0.50620
C	1.86900	0.49310	-0.43520
H	2.77830	-0.10550	-0.46950
H	1.83630	1.12560	-1.32280
H	1.92040	1.13280	0.44840

H_3C-CHOH-CHOH-$CH_3\cdots(H_2O)$

E(RM062X)=-385.319255993

C	0.14170	-0.51930	0.71120
C	0.90490	0.30640	-0.31100
O	-0.96690	0.24220	1.20880
H	-0.63210	1.11500	1.44780
O	1.30400	1.49550	0.37970
H	1.69100	2.10120	-0.26040
O	-2.73910	0.68650	-0.95630
H	-2.13620	0.53310	-0.20850
H	-2.78180	-0.16110	-1.40840
C	-0.41200	-1.80530	0.13960
H	-0.99050	-1.60680	-0.76490
H	0.39160	-2.49700	-0.10490
H	-1.06150	-2.28290	0.87190
C	2.10920	-0.42170	-0.87410
H	1.80390	-1.26580	-1.49070
H	2.69260	0.25770	-1.49580
H	2.74620	-0.78560	-0.06630
H	0.21260	0.57550	-1.11560
H	0.81750	-0.73810	1.54440

H_3C-CHOH-CHOH-$CH_3\cdots(H_2O)_2$

E(RM062X)=-461.76159629

O	-0.80090	1.63690	0.37330
H	-1.46960	1.67890	1.06680
H	1.11150	1.77510	0.29600
O	2.04140	1.66540	0.03980
H	2.16360	2.25790	-0.70880
H	2.12960	-0.08310	-0.66620
O	-0.41480	-1.94340	-0.20020
O	2.16740	-0.98100	-1.04310
H	0.47470	-1.74540	-0.54120
H	2.79570	-1.45310	-0.48780
C	-0.79740	-0.82190	0.59660
C	-0.93680	0.39830	-0.32940
H	-0.09110	0.38220	-1.01960
H	-1.78270	-1.06880	0.99970
C	-2.23760	0.36190	-1.10610
H	-2.27870	1.17400	-1.83070
H	-2.33760	-0.58500	-1.63620
H	-3.07900	0.46160	-0.41740
C	0.16980	-0.61910	1.74930
H	-0.18520	0.15430	2.42870
H	0.25780	-1.55060	2.30810
H	1.15880	-0.33630	1.38800

H_3C-CHOH-CHOH-$CH_3\cdots(H_2O)_3$

E(RM062X)=-538.208542841

O	-0.60430	1.93160	-0.25500
H	-1.33720	2.34170	0.22030
H	1.12300	2.00610	0.28220
O	2.08770	1.93420	0.40550
H	2.19930	1.67780	1.32650
H	2.38420	0.35150	-0.45710
O	2.57460	-0.48950	-0.91550
H	2.33240	-0.32920	-1.83340
H	1.44310	-1.84150	-0.48640
O	-1.56410	-1.52340	0.54250
O	0.86390	-2.61610	-0.34890
H	-0.73970	-1.94130	0.23100
H	1.21410	-3.05310	0.43350
C	-1.27020	-0.15470	0.80200
C	-0.93680	0.56050	-0.50980
C	-2.06030	0.47630	-1.52320
H	-2.96740	0.92380	-1.11100
H	-1.78720	1.01520	-2.42960
H	-2.27340	-0.55810	-1.78590
C	-0.16270	-0.02870	1.83430
H	-0.00560	1.01020	2.12160

H	-0.42750	-0.59540	2.72650
H	0.77450	-0.42460	1.43480
H	-0.02290	0.11910	-0.91830
H	-2.19220	0.28260	1.19700

H_3C-CHOH-CHOH-$CH_3\cdots(H_2O)_4$
E(RM062X)=-614.652852914

O	0.78250	1.58080	1.21700
H	1.68130	1.86880	1.41610
H	-0.51180	2.46160	0.30470
O	-1.29090	2.74740	-0.20630
H	-1.85890	3.19500	0.42870
H	-2.09880	1.17640	-0.59060
O	-2.56190	0.33990	-0.79400
H	-2.01350	-0.09010	-1.45870
H	-2.34580	-0.83480	0.59350
O	-2.16270	-1.61260	1.15470
H	-1.59570	-1.28780	1.86180
H	-1.04250	-2.22280	-0.19310
O	1.97150	-1.20720	-0.85470
O	-0.50160	-2.50560	-0.95340
H	1.10410	-1.64600	-0.93380
H	-0.97330	-2.18770	-1.73000
C	1.74970	0.14620	-0.47560
C	0.82780	0.22890	0.74460
H	2.72660	0.53880	-0.17660
C	1.20590	0.94980	-1.64370
H	1.09320	2.00130	-1.38220
H	1.88120	0.87720	-2.49550
H	0.22890	0.55850	-1.93980
C	1.22530	-0.71280	1.86310
H	0.57950	-0.55170	2.72660
H	1.13140	-1.75170	1.55050
H	2.26030	-0.53180	2.16140
H	-0.19400	0.01320	0.42060

Hydrolysis of 2,2,3-trimethyloxirane at 333 K. The substitution reaction occurs on the most substituted carbon atom.

H_3C-CH-O-C-$(CH_3)_2\cdots H_2O$
E(RM062X)=-348.156928073

C	0.42740	0.61660	-0.06070
C	0.49630	-0.79540	-0.46460
H	-0.17420	-1.08500	-1.26820
O	-2.99080	-0.63590	0.27870
H	-3.24580	0.15130	-0.21130
O	-0.22050	-0.41090	0.72950
H	-2.03700	-0.52660	0.43590
C	-0.53110	1.53040	-0.77380

H	0.00570	2.12470	-1.51370
H	-1.31100	0.96380	-1.28060
H	-0.99360	2.21560	-0.06140
C	1.57690	1.30710	0.61720
H	1.19760	2.09020	1.27520
H	2.17570	0.62030	1.20910
H	2.21580	1.77700	-0.13100
C	1.68290	-1.68900	-0.28160
H	1.35170	-2.71470	-0.11850
H	2.29460	-1.67490	-1.18420
H	2.29630	-1.38580	0.56320

H_3C-CH-O-C-$(CH_3)_2\cdots(H_2O)_3$

E(RM062X)=-501.044334207

O	1.43230	2.54120	-0.25270
H	0.72890	2.54490	0.40320
H	1.90550	1.70300	-0.10820
O	2.98930	0.19040	0.06300
H	3.36390	0.16730	-0.82330
H	2.48690	-0.64260	0.14140
O	-1.02160	-1.22870	0.39220
O	1.59670	-2.24570	0.28010
H	0.65550	-1.99700	0.31470
H	1.79740	-2.59620	1.15370
C	-0.68540	0.12000	0.78710
C	-1.19980	-0.15150	-0.56310
H	0.38970	0.25920	0.85960
C	-0.23950	-0.19240	-1.71990
H	-0.50620	-1.00870	-2.39330
H	-0.29740	0.74060	-2.28080
H	0.78510	-0.33230	-1.37880
C	-2.62790	0.12860	-0.93790
H	-2.71190	1.14140	-1.33310
H	-2.94280	-0.56380	-1.71990
H	-3.30210	0.02440	-0.09230
C	-1.47220	0.73140	1.90360
H	-1.13120	0.33600	2.86060
H	-1.30760	1.81010	1.90950
H	-2.53760	0.53940	1.80760

H_3C-CH-O-C-$(CH_3)_2\cdots(H_2O)_4$

E(RM062X)=-577.489500299

O	-2.08460	2.30740	-0.11050
H	-2.41090	1.50060	0.29780
H	-1.11470	2.24920	-0.06040
O	0.69690	2.63790	-0.04580
H	0.79670	3.27120	0.67180
H	1.42670	2.00090	0.07580
O	2.92790	1.00490	0.28760

H	3.49930	1.32520	-0.41760
H	2.81020	0.05180	0.10510
O	-0.13440	-1.81450	0.18650
O	2.61260	-1.71080	-0.17330
H	1.64980	-1.82570	-0.06290
H	3.00780	-2.15180	0.58540
C	-0.44820	-0.56390	0.84070
C	-0.86470	-0.80200	-0.55110
H	0.43090	0.06370	0.96140
C	-0.07360	-0.16670	-1.66180
H	0.00480	-0.85590	-2.50420
H	-0.57990	0.73540	-2.00620
H	0.92790	0.10070	-1.32620
C	-1.34410	-0.63520	2.03800
H	-0.77560	-0.96660	2.90720
H	-1.74110	0.35720	2.25810
H	-2.17350	-1.32080	1.88500
C	-2.27320	-1.18340	-0.91100
H	-2.77870	-1.70150	-0.10050
H	-2.84240	-0.28980	-1.17010
H	-2.26080	-1.83620	-1.78520

H_3C-CH-O-C-$(CH_3)_2\cdots(H_2O)_5$

E(RM062X)=-653.934123831

O	1.69660	-2.48210	-0.97200
H	2.14630	-2.15750	-0.18650
H	0.74930	-2.45360	-0.75000
O	-1.08450	-2.59380	-0.61080
H	-1.43190	-2.27040	-1.44850
H	-1.57930	-2.10120	0.06810
O	-2.74900	-1.08600	1.12240
H	-2.23340	-0.65730	1.81280
H	-2.77600	-0.44160	0.38860
O	-2.65370	0.52710	-1.15310
H	-1.96830	0.03800	-1.62160
H	-2.20920	1.33610	-0.83170
O	0.79420	1.53110	0.89690
O	-1.44530	2.82930	-0.13730
H	-0.64060	2.46070	0.27230
H	-1.99330	3.12210	0.59780
C	0.46050	0.13430	0.72700
C	1.49360	0.75970	-0.11270
H	-0.50580	0.00680	0.24780
C	1.13710	1.13160	-1.52600
H	1.62930	2.06470	-1.80490
H	1.47860	0.35170	-2.20720
H	0.05970	1.25030	-1.64140
C	2.96300	0.58430	0.14710
H	3.17090	0.33610	1.18450

H	3.36140	-0.20210	-0.49470
H	3.48490	1.51040	-0.09910
C	0.70300	-0.77170	1.89370
H	-0.04220	-0.58400	2.66850
H	0.59800	-1.81030	1.57570
H	1.69110	-0.63240	2.32600

$[H_3C\text{-}CH\text{-}O\text{-}C\text{-}(CH_3)_2\cdots H_2O]^{\ddagger}$
E(RM062X)=-348.156928073

C	-0.23330	0.57600	0.05920
C	0.76680	-0.41910	-0.41890
H	0.70970	-0.41790	-1.51840
O	-1.80370	-1.12340	-0.27760
H	-1.92490	-1.16680	-1.23180
O	0.59970	-1.67200	0.12560
H	-0.89510	-1.57910	-0.09390
C	-0.63120	1.68360	-0.81720
H	-0.59040	2.62960	-0.27610
H	-0.04930	1.71420	-1.73460
H	-1.68380	1.51820	-1.06950
C	-0.58740	0.64620	1.47810
H	-1.57040	1.09020	1.61980
H	-0.48930	-0.30790	1.98430
H	0.14180	1.35200	1.90210
C	2.12220	0.24540	-0.04740
H	2.90060	-0.39070	-0.46510
H	2.22930	1.24870	-0.45970
H	2.23170	0.27980	1.03580

$[H_3C\text{-}CH\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_3]^{\ddagger}$
E(RM062X)=-500.992374234

O	0.57830	2.02100	-0.61490
H	0.96590	1.87850	-1.48640
H	-0.38320	1.89810	-0.73780
O	-2.24030	1.41510	-0.71980
H	-2.65280	2.00750	-0.08300
H	-2.35690	0.52340	-0.34240
O	0.08360	-1.81990	0.35450
O	-2.46400	-1.25270	0.42050
H	-1.50240	-1.55790	0.44160
H	-2.90150	-1.82160	-0.21920
C	0.36870	-0.75380	-0.50970
C	0.88000	0.16170	0.54920
H	-0.53520	-0.33420	-0.96180
C	-0.01610	0.62270	1.63450
H	0.23560	0.05420	2.53290
H	0.20720	1.66530	1.85710
H	-1.06760	0.49350	1.40510
C	2.33170	0.26120	0.79810

H	2.88180	0.46260	-0.11820
H	2.55720	0.99920	1.56310
H	2.65030	-0.72180	1.16080
C	1.34950	-1.10150	-1.61320
H	0.87640	-1.81710	-2.28510
H	1.62960	-0.22150	-2.19540
H	2.25160	-1.55880	-1.20730

$[H_3C\text{-}CH\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_4]^{\ddagger}$

E(RM062X)=-577.443353177

O	-1.29200	1.94860	-0.19430
H	-1.78490	2.04750	0.62850
H	-0.35950	2.18370	0.02240
O	1.31760	2.51870	0.24310
H	1.45740	2.91930	1.10710
H	1.87200	1.71130	0.24100
O	3.02950	0.35470	0.21030
H	3.63180	0.55450	-0.51310
H	2.64530	-0.52490	-0.00870
O	-0.43500	-1.88010	0.27070
O	1.99740	-2.09460	-0.35690
H	1.00080	-2.04110	-0.10170
H	2.39900	-2.69210	0.28070
C	-0.55420	-0.56440	0.75460
C	-1.10970	-0.13000	-0.54540
H	0.42270	-0.09510	0.92880
C	-0.16890	0.03990	-1.68790
H	-0.19600	-0.86100	-2.30200
H	-0.50270	0.86540	-2.31340
H	0.84950	0.21480	-1.34680
C	-1.41600	-0.44690	1.99140
H	-0.90590	-0.94800	2.81430
H	-1.57620	0.59330	2.27840
H	-2.38160	-0.93010	1.84560
C	-2.55010	-0.32930	-0.86130
H	-3.18900	-0.03230	-0.03330
H	-2.81650	0.22830	-1.75610
H	-2.71420	-1.38800	-1.06330

$[H_3C\text{-}CH\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_5]^{\ddagger}$

E(RM062X)=-653.888047745

O	1.45360	-1.82130	-0.86700
H	1.88960	-2.30250	-0.15350
H	0.49830	-2.05360	-0.79340
O	-1.18550	-2.42160	-0.78950
H	-1.53510	-2.01990	-1.59220
H	-1.67360	-1.99160	-0.06160
O	-2.76200	-1.07330	1.10720
H	-2.18690	-0.76460	1.81470

H	-2.78160	-0.34190	0.45710
O	-2.74050	0.77060	-0.95480
H	-2.28440	0.24170	-1.61730
H	-2.10260	1.47880	-0.70670
O	0.76630	1.55080	1.04980
O	-1.04670	2.76650	-0.21890
H	-0.29960	2.30580	0.31820
H	-1.54870	3.27990	0.42110
C	0.51490	0.19110	0.79310
C	1.53700	0.19960	-0.27590
H	-0.47800	0.03140	0.35410
C	1.13380	0.72450	-1.61150
H	1.28070	1.80500	-1.61890
H	1.77040	0.30140	-2.38500
H	0.08750	0.50690	-1.82280
C	2.99280	0.19050	0.03680
H	3.21730	-0.29630	0.98150
H	3.52600	-0.30520	-0.77190
H	3.34630	1.22100	0.07200
C	0.69270	-0.71610	1.98890
H	-0.04650	-0.43860	2.74230
H	0.53110	-1.76240	1.72440
H	1.68080	-0.60650	2.43450

H_3C-CHOH-COH-$(CH_3)_2$

E(RM062X)=-348.186276427

C	0.62040	-0.01380	0.00780
C	-0.84700	0.02270	-0.45550
H	-0.82670	0.01600	-1.55210
O	1.22930	1.21200	-0.44210
H	1.26070	1.19090	-1.40600
O	-1.47320	1.22800	-0.01610
H	-0.85910	1.94770	-0.20450
C	1.35340	-1.19360	-0.61180
H	0.97790	-2.13980	-0.22540
H	1.23510	-1.18960	-1.69730
H	2.41550	-1.12490	-0.37760
C	0.75810	-0.01180	1.51940
H	1.81150	0.07170	1.78670
H	0.21920	0.82620	1.96010
H	0.37220	-0.93820	1.94160
C	-1.69960	-1.12720	0.03580
H	-2.70790	-1.02900	-0.36530
H	-1.29800	-2.08400	-0.29280
H	-1.76180	-1.12430	1.12400

H_3C-CHOH-COH-$(CH_3)_2\cdots(H_2O)_2$

E(RM062X)=-501.072409473

O	-0.62600	-1.62450	-0.59730

H	-1.19410	-1.52200	-1.36950
H	1.29470	-1.53040	-0.92120
O	2.24580	-1.34510	-0.99800
H	2.67080	-2.00690	-0.44290
H	2.53420	0.27140	0.02460
O	-0.14400	1.81970	0.51000
O	2.63910	1.06430	0.57860
H	0.77500	1.70080	0.79500
H	3.08410	1.70410	0.01410
C	-0.41090	0.77050	-0.41690
C	-0.86440	-0.52390	0.30450
H	0.51810	0.52270	-0.93490
C	-0.00490	-0.81290	1.52430
H	-0.16690	-0.06170	2.29450
H	-0.28130	-1.78600	1.93010
H	1.05490	-0.83160	1.27300
C	-2.33300	-0.49020	0.69800
H	-2.97660	-0.47770	-0.18160
H	-2.57860	-1.37050	1.29200
H	-2.54540	0.39920	1.29280
C	-1.40970	1.28940	-1.43310
H	-0.95770	2.09540	-2.00930
H	-1.71440	0.50530	-2.12710
H	-2.30000	1.67520	-0.93680

H_3C-CHOH-COH-$(CH_3)_2\cdots(H_2O)_3$
E(RM062X)=-577.519581596

O	-1.09390	1.62950	-0.47850
H	-1.82350	1.92220	0.07900
H	0.49580	2.17630	0.19130
O	1.37550	2.45600	0.50900
H	1.30880	2.43610	1.46920
H	2.51850	1.10510	0.15810
O	3.17500	0.39730	0.00460
H	3.50570	0.55580	-0.88530
H	2.41730	-1.23530	-0.12360
O	-0.56790	-1.82970	0.64640
O	2.05950	-2.14150	-0.20310
H	0.32310	-2.01080	0.29640
H	2.50450	-2.64640	0.48500
C	-0.71020	-0.41750	0.75520
C	-1.13880	0.19290	-0.59910
H	0.26460	0.02250	0.99550
C	-0.11670	-0.14500	-1.67040
H	-0.09310	-1.21730	-1.85620
H	-0.37880	0.36070	-2.59950
H	0.87910	0.17970	-1.36180
C	-1.67940	-0.14220	1.88930
H	-1.25480	-0.50150	2.82580

H	-1.88360	0.92280	2.00190
H	-2.62280	-0.66190	1.72040
C	-2.53650	-0.23510	-1.01650
H	-3.28590	0.15920	-0.32890
H	-2.75360	0.14210	-2.01560
H	-2.61730	-1.32160	-1.02970

H_3C-CHOH-COH-$(CH_3)_2\cdots(H_2O)_4$
E(RM062X)=-653.96426289

O	1.33150	-1.36320	-1.05300
H	1.75300	-2.05040	-0.52330
H	-0.40180	-1.97540	-0.96580
O	-1.28660	-2.37680	-0.88150
H	-1.78300	-2.04800	-1.63820
H	-2.16280	-1.61050	0.52490
O	-2.75790	-1.09030	1.09860
H	-2.19370	-0.74000	1.79530
H	-2.71600	0.18460	-0.26010
O	-2.63490	0.77340	-1.03270
H	-2.03470	0.30960	-1.62640
H	-1.64350	2.15770	-0.40130
O	0.71520	1.32160	1.38490
O	-1.09260	2.88680	-0.05560
H	0.16390	1.95480	0.89230
H	-1.64550	3.32890	0.59630
C	0.57660	0.05000	0.75870
C	1.56460	-0.08630	-0.42250
H	-0.42850	-0.02700	0.32880
C	1.25030	0.95540	-1.48150
H	1.38670	1.95910	-1.08190
H	1.91580	0.82900	-2.33520
H	0.21820	0.85300	-1.82280
C	3.01700	0.00270	0.01640
H	3.27910	-0.82640	0.67490
H	3.66710	-0.03330	-0.85780
H	3.20020	0.93640	0.54610
C	0.74140	-1.01690	1.82360
H	-0.02720	-0.89080	2.58630
H	0.64010	-2.01810	1.40500
H	1.71460	-0.93420	2.30860

Hydrolysis of 2,2,3-trimethyloxirane at 333 K. The substitution reaction occurs on the least substituted carbon atom.

H_3C-CH-O-C-$(CH_3)_2\cdots H_2O$
E(RM062X)=-348.156928257

C	-0.42730	-0.61670	-0.06080
C	-0.49610	0.79530	-0.46480
H	0.17420	1.08450	-1.26860

O	2.99040	0.63570	0.27910
H	3.24460	-0.15100	-0.21220
O	0.22100	0.41090	0.72910
H	2.03640	0.52720	0.43610
C	0.53050	-1.53080	-0.77410
H	0.99260	-2.21650	-0.06200
H	-0.00680	-2.12460	-1.51410
H	1.31070	-0.96460	-1.28080
C	-1.57670	-1.30670	0.61790
H	-2.21610	-1.77660	-0.13000
H	-1.19740	-2.08980	1.27590
H	-2.17510	-0.61960	1.20990
C	-1.68250	1.68920	-0.28160
H	-1.35090	2.71490	-0.11880
H	-2.29440	1.67520	-1.18410
H	-2.29570	1.38650	0.56340

H_3C-CH-O-C-$(CH_3)_2\cdots(H_2O)_2$

E(RM062X)=-424.60030088

C	-1.43460	0.05100	-0.10990
C	-0.42440	0.86420	0.58400
H	-0.55650	1.93910	0.51080
O	-0.13030	0.26890	-0.70080
H	2.30210	1.49570	-0.42070
O	3.09850	0.97120	-0.54920
H	2.78680	0.05280	-0.49990
O	1.90610	-1.63600	-0.48090
H	1.08940	-1.10690	-0.52730
H	1.95930	-1.92610	0.43530
C	0.39110	0.41050	1.75610
H	1.38510	0.85730	1.71560
H	-0.08850	0.74310	2.67730
H	0.49820	-0.67120	1.78970
C	-1.72150	-1.36990	0.28740
H	-2.55030	-1.39300	0.99550
H	-2.01520	-1.94160	-0.59410
H	-0.85840	-1.85180	0.73980
C	-2.55040	0.74760	-0.83750
H	-2.26310	1.76250	-1.10740
H	-2.80760	0.19720	-1.74360
H	-3.43680	0.78900	-0.20390

H_3C-CH-O-C-$(CH_3)_2\cdots(H_2O)_3$

E(RM062X)=-501.044913462

O	-1.48270	2.51450	-0.33460
H	-0.57770	2.30000	-0.57870
H	-1.91660	1.65430	-0.19470
O	-2.98130	0.17290	0.17390
H	-3.24700	0.32480	1.08630

H	-2.48440	-0.66710	0.19220
O	0.98820	-1.22730	0.36640
O	-1.59390	-2.26740	0.17390
H	-0.66010	-1.98820	0.19480
H	-1.73770	-2.57670	-0.72640
C	1.20230	-0.10900	-0.53180
C	0.68130	0.10850	0.82660
C	0.25110	-0.06890	-1.69730
H	-0.78150	-0.18290	-1.36950
H	0.35110	0.88170	-2.22330
H	0.49330	-0.86800	-2.39990
C	2.64070	0.15460	-0.87930
H	2.93400	-0.47050	-1.72390
H	2.76390	1.19700	-1.17450
H	3.30570	-0.05670	-0.04620
C	1.47600	0.63380	1.98050
H	1.33170	1.71200	2.05810
H	1.12650	0.18180	2.90900
H	2.53790	0.42850	1.87240
H	-0.39020	0.27480	0.89530

H_3C-CH-O-C-$(CH_3)_2\cdots(H_2O)_4$
E(RM062X)=-577.489947904

O	1.23030	2.75910	0.19150
H	1.74420	1.95340	0.08580
H	0.31690	2.51570	-0.04420
O	-1.46330	2.40540	-0.51150
H	-1.37790	2.19140	-1.44600
H	-1.93610	1.64410	-0.12340
O	-2.94310	0.36070	0.67980
H	-2.67470	0.43260	1.60150
H	-2.65660	-0.53100	0.40220
O	0.55970	-1.74320	0.22390
O	-2.16190	-2.18490	-0.17880
H	-1.19340	-2.10980	-0.09120
H	-2.32530	-2.13160	-1.12620
C	1.06880	-0.62960	-0.54970
C	0.59690	-0.43210	0.83160
C	2.53130	-0.70790	-0.88800
H	2.67190	-1.35670	-1.75360
H	2.90090	0.28480	-1.15110
H	3.12220	-1.09640	-0.06340
C	1.47510	-0.27440	2.03410
H	2.44360	-0.74870	1.89680
H	1.62730	0.78510	2.24150
H	0.99130	-0.71980	2.90370
C	0.17580	-0.21620	-1.68820
H	0.48860	0.75860	-2.06610
H	0.25510	-0.93770	-2.50310

H	-0.86390	-0.15210	-1.36850
H	-0.39460	0.00290	0.92660

H_3C-CH-O-C-$(CH_3)_2\cdots(H_2O)_5$

E(RM062X)=-653.933101685

O	1.05770	-2.90220	-0.53940
H	1.52630	-2.35030	0.09330
H	0.19960	-2.46280	-0.67940
O	-1.48360	-1.85020	-1.12430
H	-1.35850	-0.95550	-1.45850
H	-1.99020	-1.72840	-0.30180
O	-3.12470	-1.21430	1.11400
H	-2.55190	-1.09930	1.87860
H	-3.14190	-0.34290	0.67360
O	-3.18390	1.03280	-0.51940
H	-3.16060	0.57810	-1.36740
H	-2.39720	1.61220	-0.51800
O	1.40270	1.60030	0.09270
O	-1.03750	2.79710	-0.52270
H	-0.19210	2.39290	-0.25240
H	-1.24440	3.43330	0.16900
C	1.32120	0.31760	0.76040
C	1.50710	0.39390	-0.69710
C	2.79920	0.16200	-1.41650
H	3.65850	0.40920	-0.79860
H	2.86650	-0.88500	-1.71380
H	2.83460	0.77090	-2.32010
C	-0.04680	-0.01260	1.29050
H	-0.11140	-1.08200	1.50090
H	-0.23430	0.52980	2.21900
H	-0.81630	0.24700	0.56430
H	0.61440	0.21530	-1.29060
C	2.45950	0.01070	1.69230
H	2.28230	0.48860	2.65660
H	2.51660	-1.06650	1.85810
H	3.41280	0.35770	1.30300

$[H_3C$-CH-O-C-$(CH_3)_2\cdots H_2O]^{\ddagger}$

E(RM062X)=-348.082920956

C	-0.67500	-0.21930	0.05350
C	0.33940	0.61020	-0.65960
H	0.76160	0.25240	-1.59350
O	2.27030	-0.78340	0.14340
H	2.24520	-1.59470	-0.37350
O	0.01600	-0.50880	1.23820
H	1.42250	-0.80070	0.71180
C	-1.00140	-1.47380	-0.74920
H	-1.69000	-2.09580	-0.17830
H	-1.46430	-1.22020	-1.70430

H	-0.09130	-2.04420	-0.94050
C	-1.94200	0.60110	0.31070
H	-2.43760	0.88730	-0.61730
H	-2.61900	-0.02690	0.89130
H	-1.71650	1.49540	0.88900
C	0.75160	1.92080	-0.21960
H	1.80460	2.11020	-0.41910
H	0.20200	2.57200	-0.92770
H	0.45720	2.16910	0.79370

$[H_3C\text{-}CH\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_2]^{\ddagger}$

E(RM062X)=-424.527087977

C	0.92620	-0.42320	-0.13490
C	0.24500	0.65150	0.61900
H	-0.50950	0.30230	1.31700
O	-0.12550	-1.08810	-0.76660
H	-2.30590	1.94140	0.10780
O	-2.03630	1.29250	-0.54960
H	-2.36450	0.43780	-0.21700
O	-2.40680	-1.33930	0.35890
H	-1.47860	-1.29880	-0.05880
H	-2.94860	-1.83910	-0.25830
C	1.60880	-1.30340	0.93240
H	2.04710	-2.15040	0.40170
H	2.39780	-0.77440	1.46840
H	0.87180	-1.67640	1.64280
C	1.95600	0.09140	-1.13220
H	2.74950	0.65690	-0.64140
H	2.40240	-0.76470	-1.63670
H	1.47820	0.72470	-1.87980
C	0.58790	2.04870	0.61570
H	-0.17020	2.69430	1.04420
H	1.45900	2.03470	1.30580
H	0.97660	2.40040	-0.33740

$[H_3C\text{-}CH\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_3]^{\ddagger}$

E(RM062X)=-500.992683595

O	0.07070	2.06910	0.49110
H	-0.38740	2.00760	1.33940
H	0.99930	1.80680	0.66080
O	2.64810	0.93630	0.41970
H	3.18660	1.45930	-0.18290
H	2.49790	0.09090	-0.04270
O	-0.63940	-1.48640	-0.71790
O	2.00360	-1.57720	-0.89200
H	1.00430	-1.61450	-0.82260
H	2.32290	-2.17790	-0.21170
C	-0.88670	-0.57650	0.33050
C	-0.43650	0.49160	-0.59080

C	-0.02570	-0.81360	1.56160
H	1.03530	-0.79210	1.32360
H	-0.22660	-0.07160	2.33610
H	-0.26950	-1.79850	1.96380
C	-2.35490	-0.50570	0.71890
H	-2.62080	-1.40960	1.26810
H	-2.54890	0.35430	1.36300
H	-2.99310	-0.43950	-0.16060
C	-1.37010	1.17410	-1.52850
H	-2.19330	1.63740	-0.98830
H	-0.84300	1.92730	-2.10750
H	-1.78480	0.43710	-2.21530
H	0.59890	0.42930	-0.88000

$[H_3C\text{-}CH\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_4]^{\ddagger}$

E(RM062X)=-577.443033096

O	0.44700	2.14990	0.33540
H	1.08580	2.35670	-0.35820
H	-0.44440	2.16010	-0.09740
O	-2.03230	2.05270	-0.65950
H	-1.93110	1.84280	-1.59380
H	-2.33940	1.21790	-0.24660
O	-2.93150	-0.21900	0.60860
H	-2.84110	-0.00590	1.54280
H	-2.37630	-1.01910	0.47280
O	0.96290	-1.64480	0.18060
O	-1.44990	-2.48520	0.21280
H	-0.48840	-2.15180	0.16190
H	-1.67930	-2.73780	-0.68680
C	1.12410	-0.42550	-0.51280
C	0.72020	0.22010	0.74900
C	2.55370	-0.18160	-0.95820
H	2.78240	-0.84030	-1.79680
H	2.69270	0.85050	-1.28680
H	3.25620	-0.39340	-0.15370
C	1.66400	0.45240	1.88100
H	2.53760	1.01060	1.54950
H	1.16570	1.00040	2.67610
H	1.99700	-0.50390	2.27900
C	0.14380	-0.24940	-1.66000
H	0.25970	0.72990	-2.12750
H	0.33620	-1.01600	-2.41260
H	-0.88380	-0.35250	-1.31070
H	-0.33470	0.12630	0.97260

$[H_3C\text{-}CH\text{-}O\text{-}C\text{-}(CH_3)_2\cdots(H_2O)_5]^{\ddagger}$

E(RM062X)=-653.885388537

O	1.04320	-2.10750	-0.56450
H	1.30450	-2.37850	0.32460

H	0.05410	-2.13320	-0.58220
O	-1.61750	-2.06100	-0.86470
H	-1.70170	-1.34050	-1.49940
H	-2.11770	-1.75740	-0.08320
O	-3.19580	-0.99060	1.19780
H	-2.62970	-0.82580	1.95850
H	-3.15230	-0.17180	0.66630
O	-3.06700	1.08430	-0.64280
H	-3.10550	0.59400	-1.47010
H	-2.22690	1.59100	-0.67980
O	1.40970	1.64650	0.10240
O	-0.80250	2.61320	-0.75690
H	0.05860	2.21760	-0.38600
H	-1.00180	3.37060	-0.19870
C	1.30400	0.36920	0.69160
C	1.44760	-0.16310	-0.67560
C	2.77000	-0.32550	-1.34610
H	3.44070	-0.92730	-0.73550
H	2.64200	-0.79710	-2.31660
H	3.22380	0.65230	-1.49610
C	-0.05030	0.11260	1.32860
H	-0.11620	-0.90240	1.72460
H	-0.19660	0.81530	2.15100
H	-0.84830	0.25800	0.60110
H	0.57330	-0.02150	-1.29710
C	2.44140	0.05940	1.64610
H	2.30240	0.63170	2.56400
H	2.45730	-1.00160	1.90410
H	3.40220	0.33150	1.21210

H_3C-CHOH-COH-$(CH_3)_2$

E(RM062X)=-348.185584275

C	-0.62300	0.05880	0.02620
C	0.82440	-0.08060	-0.48480
H	0.78870	-0.12600	-1.57670
O	1.40070	-1.29100	0.01960
H	0.99060	-2.04120	-0.42180
O	-0.62560	-0.03010	1.45670
H	-0.16740	-0.84750	1.68760
C	-1.49590	-1.05150	-0.54920
H	-2.51260	-0.95010	-0.17040
H	-1.52250	-0.99570	-1.63790
H	-1.12760	-2.03660	-0.25860
C	-1.20200	1.41720	-0.32680
H	-1.11090	1.60130	-1.39770
H	-2.25890	1.44880	-0.06180
H	-0.68730	2.21300	0.20910
C	1.74190	1.04480	-0.05420
H	2.75940	0.82670	-0.37550

H	1.43880	1.98820	-0.50350
H	1.73640	1.15580	1.03040

H_3C-CHOH-COH-$(CH_3)_2\cdots(H_2O)$

E(RM062X)=-424.629794263

C	-0.83920	0.35080	-0.05610
C	-0.21990	-0.92330	0.55930
H	-0.92360	-1.28780	1.31190
O	-0.15990	0.73120	-1.25730
H	0.87060	-0.09220	1.97840
O	1.03180	-0.65190	1.21140
H	2.23320	0.25280	0.15780
O	2.64190	0.85150	-0.49330
H	0.77560	0.88830	-1.05290
H	3.06840	0.27120	-1.13150
C	0.07090	-2.01280	-0.45030
H	0.42130	-2.90620	0.06470
H	-0.81810	-2.27250	-1.02100
H	0.84610	-1.68370	-1.14280
C	-2.28110	0.07550	-0.45530
H	-2.87080	-0.20110	0.41820
H	-2.71320	0.97570	-0.89190
H	-2.34450	-0.72680	-1.18900
C	-0.78570	1.50220	0.94340
H	0.24400	1.81250	1.12590
H	-1.33270	2.35680	0.54600
H	-1.23710	1.21210	1.89390

H_3C-CHOH-COH-$(CH_3)_2\cdots(H_2O)_2$

E(RM062X)=-501.071896056

O	-0.14910	1.78590	0.51780
H	-0.93490	1.96310	1.04820
H	1.76350	1.42430	0.69020
O	2.65480	1.08140	0.52200
H	3.07110	1.73870	-0.04470
H	2.42050	-0.53210	-0.46620
O	-0.61220	-1.62350	-0.67950
O	2.28300	-1.35600	-0.96650
H	0.34410	-1.63750	-0.85400
H	2.58700	-2.05310	-0.37640
C	-0.84790	-0.57330	0.26850
C	-0.44900	0.75240	-0.42480
C	-0.01120	-0.81690	1.51990
H	1.05480	-0.73210	1.31080
H	-0.26550	-0.10640	2.30500
H	-0.21410	-1.82300	1.88730
C	-2.32440	-0.62470	0.62180
H	-2.53640	-1.52710	1.19530
H	-2.59900	0.23920	1.22980

H	-2.94480	-0.62980	-0.27320
C	-1.45700	1.24500	-1.44630
H	-2.37410	1.57300	-0.95550
H	-1.03990	2.08690	-1.99710
H	-1.70630	0.45620	-2.15570
H	0.50020	0.56270	-0.92780

H_3C-CHOH-COH-$(CH_3)_2\cdots(H_2O)_3$

E(RM062X)=-577.518941058

O	-0.39330	-1.79520	0.55710
H	-1.20520	-2.27890	0.36590
H	1.19190	-2.08730	-0.23730
O	2.11580	-2.15060	-0.54350
H	2.07560	-1.94500	-1.48320
H	2.71420	-0.55950	0.10860
O	3.05840	0.29870	0.42240
H	3.31030	0.15140	1.33930
H	1.95020	1.71620	0.33890
O	-1.20980	1.69190	-0.24840
O	1.41600	2.53390	0.31500
H	-0.30640	1.99710	-0.04530
H	1.69050	2.98390	-0.49000
C	-1.14670	0.28860	-0.52320
C	-0.70900	-0.41640	0.78050
C	-2.53770	-0.12650	-0.97220
H	-2.76170	0.33180	-1.93560
H	-2.60310	-1.20900	-1.08930
H	-3.29130	0.19410	-0.25420
C	-1.71020	-0.29560	1.91320
H	-2.61040	-0.86950	1.68760
H	-1.27730	-0.68570	2.83330
H	-1.99360	0.74270	2.07680
C	-0.12810	0.03510	-1.62920
H	-0.12640	-1.01150	-1.93220
H	-0.38130	0.64460	-2.49700
H	0.87730	0.30230	-1.29630
H	0.24010	0.04040	1.07520

H_3C-CHOH-COH-$(CH_3)_2\cdots(H_2O)_4$

E(RM062X)=-653.962809013

O	-0.48080	-1.62480	0.85380
H	-1.06480	-2.32890	0.54750
H	1.23490	-1.92720	0.30290
O	2.14550	-2.18280	0.06550
H	2.61220	-2.24100	0.90570
H	2.95990	-0.78700	-0.76550
O	3.43400	0.02990	-1.01500
H	2.92860	0.39920	-1.74580
H	2.65650	0.70740	0.56520

O	2.17030	0.88260	1.39050
H	1.68460	0.06580	1.55280
H	0.96600	2.16370	0.81110
O	-1.78530	1.44430	-0.66680
O	0.36850	2.87280	0.50770
H	-1.07210	1.97510	-0.26790
H	0.80730	3.24980	-0.26150
C	-1.34500	0.08170	-0.69630
C	-1.17930	-0.37740	0.76830
C	-2.47800	-0.45910	1.54700
H	-3.09790	-1.27550	1.17250
H	-2.26600	-0.64520	2.59900
H	-3.04110	0.46910	1.46520
C	-0.00950	-0.00460	-1.42720
H	0.28660	-1.04030	-1.58900
H	-0.10050	0.48320	-2.39810
H	0.77290	0.49670	-0.85430
H	-0.51440	0.34780	1.24300
C	-2.41190	-0.70480	-1.43790
H	-2.42820	-0.40320	-2.48550
H	-2.20310	-1.77480	-1.39590
H	-3.39750	-0.52520	-1.01050

Hydrolysis of 2,2,3,3-tetramethyloxirane at 333 K.

$(H_3C)_2$-C-O-C-$(CH_3)_2\cdots H_2O$
E(RM062X)=-387.466416169

C	0.62670	0.69639	0.08641
C	0.39372	-0.76361	0.12489
O	-2.97932	0.23700	-0.73339
H	-3.19826	-0.06067	0.15457
O	-0.17403	0.04891	-0.93430
H	-2.00799	0.19509	-0.77070
C	-0.13369	1.64082	0.98138
H	0.39498	1.75936	1.92787
H	-0.19467	2.62041	0.50545
H	-1.14439	1.29946	1.18464
C	1.93458	1.26756	-0.39414
H	2.58837	1.44653	0.46044
H	2.44636	0.61514	-1.09425
H	1.75529	2.22636	-0.88245
C	-0.60293	-1.38353	1.07026
H	-1.13742	-2.18459	0.55703
H	-0.06908	-1.82748	1.91139
H	-1.32831	-0.67454	1.45772
C	1.44797	-1.74080	-0.32953
H	2.13523	-1.95341	0.49027
H	0.97227	-2.67881	-0.61903
H	2.01631	-1.37108	-1.17717

$(H_3C)_2$-C-O-C-$(CH_3)_2\cdots(H_2O)_4$

E(RM062X)=-616.799302082

O	-0.56350	2.93370	0.02960
H	-1.17860	2.19420	0.00160
H	0.32080	2.52940	-0.00190
O	2.17250	2.16430	-0.06890
H	2.52230	2.61540	0.70580
H	2.51840	1.25510	-0.00700
O	3.34850	-0.41140	0.06730
H	3.86230	-0.44780	-0.74570
H	2.73130	-1.16510	0.00980
O	-1.08730	-1.58450	-0.01770
O	1.57450	-2.59280	-0.07060
H	0.65890	-2.26450	-0.02340
H	1.70100	-3.09730	0.73930
C	-1.16160	-0.34820	0.73560
C	-1.15670	-0.33430	-0.74780
C	0.07270	-0.00420	-1.55340
H	0.09620	-0.64560	-2.43630
H	0.02120	1.03030	-1.89460
H	0.99650	-0.14560	-1.00210
C	-2.43320	-0.10460	-1.51700
H	-2.34180	-0.53420	-2.51530
H	-3.29770	-0.54470	-1.03050
H	-2.60080	0.96850	-1.62830
C	-2.44370	-0.13550	1.50050
H	-2.35010	-0.56450	2.49890
H	-2.62710	0.93500	1.61140
H	-3.29970	-0.58860	1.01070
C	0.06170	-0.03160	1.55540
H	-0.00780	0.98770	1.93660
H	0.09390	-0.70670	2.41270
H	0.98780	-0.13520	1.00070

$(H_3C)_2$-C-O-C-$(CH_3)_2\cdots(H_2O)_5$

E(RM062X)=-693.244778305

O	0.89450	-2.99410	-0.21880
H	1.48190	-2.24010	-0.11130
H	0.01530	-2.61180	-0.38960
O	-1.73450	-2.16250	-0.83120
H	-1.59730	-1.39100	-1.39140
H	-2.24350	-1.81850	-0.07500
O	-3.33740	-0.88980	1.12860
H	-2.76310	-0.72190	1.88240
H	-3.23230	-0.10870	0.55120
O	-3.02570	1.14110	-0.75540
H	-2.75010	0.66700	-1.54690
H	-2.27870	1.73230	-0.53830

O	1.45950	1.55000	0.24210
O	-0.98290	2.92570	-0.07740
H	-0.13820	2.45310	0.03430
H	-1.21920	3.22270	0.80740
C	1.24790	0.24560	0.83870
C	1.61240	0.37630	-0.59280
C	0.58970	0.24360	-1.69260
H	0.88830	0.86780	-2.53620
H	0.55430	-0.79070	-2.03960
H	-0.40570	0.55020	-1.38020
C	3.01580	0.10150	-1.06800
H	3.09060	-0.93920	-1.38960
H	3.23830	0.73200	-1.92980
H	3.76360	0.28480	-0.30330
C	2.26970	-0.15450	1.87280
H	1.93700	0.17370	2.85820
H	2.36440	-1.24170	1.89650
H	3.24610	0.27910	1.68010
C	-0.16660	-0.03430	1.27530
H	-0.25780	-1.08490	1.55610
H	-0.39560	0.56960	2.15610
H	-0.89960	0.18390	0.50550

$[(H_3C)_2$-C-O-C-$(CH_3)_2 \cdots H_2O]^{\ddagger}$
E(RM062X)=-387.409564884

C	-0.43928	0.65582	0.08879
C	0.74714	-0.23089	-0.13132
O	-1.75979	-1.47705	0.01803
H	-1.61546	-1.96779	0.83265
O	0.48156	-1.20991	-1.07136
H	-0.86823	-1.54134	-0.50058
C	-0.71677	1.24581	1.40007
H	0.18706	1.76864	1.73126
H	-1.56067	1.92784	1.38386
H	-0.87462	0.44515	2.12670
C	-1.20702	1.13632	-1.05844
H	-0.90870	2.18884	-1.17353
H	-1.01250	0.58813	-1.97233
H	-2.26796	1.16268	-0.81161
C	1.29109	-0.82502	1.17148
H	2.17168	-1.41516	0.92202
H	1.57989	-0.06654	1.89798
H	0.54774	-1.48441	1.62163
C	1.77960	0.81556	-0.67246
H	1.95743	1.63550	0.02297
H	2.70744	0.26064	-0.80908
H	1.45412	1.20781	-1.63403

$[(H_3C)_2$-C-O-C-$(CH_3)_2 \cdots (H_2O)_4]^{\ddagger}$

E(RM062X)=-616.751242838

O	-0.90370	2.15260	0.05920
H	-1.34120	2.17680	0.91870
H	0.05790	2.22580	0.24680
O	1.85020	2.32740	0.35380
H	2.07600	2.64060	1.23550
H	2.31050	1.47300	0.26370
O	3.29500	-0.13930	0.05090
H	3.80660	-0.00050	-0.75240
H	2.73990	-0.92540	-0.13370
O	-0.84590	-1.79810	-0.14070
O	1.65360	-2.33170	-0.48170
H	0.67030	-2.11530	-0.32790
H	1.86620	-3.02840	0.14590
C	-1.02280	-0.60940	0.59090
C	-1.05780	0.18870	-0.67440
C	0.14950	0.31140	-1.54180
H	0.04630	-0.40500	-2.35800
H	0.16400	1.30310	-1.99060
H	1.07970	0.12480	-1.01970
C	-2.35990	0.39870	-1.36850
H	-2.22900	1.04370	-2.23370
H	-2.71560	-0.57330	-1.71400
H	-3.10820	0.81630	-0.70060
C	-2.33590	-0.61070	1.36550
H	-2.23640	-1.29690	2.20690
H	-2.57210	0.37990	1.75970
H	-3.16260	-0.95070	0.74460
C	0.12030	-0.31320	1.55330
H	-0.07320	0.59220	2.12990
H	0.19100	-1.15210	2.24770
H	1.07580	-0.20930	1.04970

$[(H_3C)_2$-C-O-C-$(CH_3)_2 \cdots (H_2O)_5]^{\ddagger}$

E(RM062X)=-693.197294494

O	1.08350	-2.18560	-0.26170
H	1.33080	-2.39400	0.64740
H	0.10170	-2.25650	-0.29150
O	-1.62110	-2.37210	-0.55270
H	-1.76100	-1.90700	-1.38460
H	-2.16850	-1.89010	0.09700
O	-3.29840	-0.93140	1.17290
H	-2.77360	-0.74490	1.95810
H	-3.20420	-0.13720	0.61060
O	-3.03130	1.12480	-0.67630
H	-2.90190	0.62050	-1.48600
H	-2.22680	1.68370	-0.59280
O	1.34040	1.72410	0.25510
O	-0.85100	2.76680	-0.51040

H	0.01550	2.33070	-0.17910
H	-1.05040	3.46740	0.11720
C	1.22840	0.41950	0.77090
C	1.46130	-0.15090	-0.59060
C	0.43470	-0.00150	-1.66390
H	0.74590	0.81710	-2.31420
H	0.42570	-0.90320	-2.27460
H	-0.56140	0.20090	-1.28460
C	2.85720	-0.36600	-1.06850
H	3.44710	-0.93180	-0.35290
H	2.85170	-0.87430	-2.02950
H	3.32240	0.61160	-1.20190
C	2.32710	0.12120	1.78330
H	2.10030	0.66070	2.70340
H	2.38810	-0.94270	2.02010
H	3.29650	0.45890	1.42180
C	-0.13310	0.12920	1.38920
H	-0.17740	-0.88280	1.79490
H	-0.28880	0.83460	2.20730
H	-0.94330	0.25670	0.67610

$(H_3C)_2$-COH-COH-$(CH_3)_2$
E(RM062X)=-387.494617041

C	-0.77434	-0.02342	0.01011
C	0.78362	0.04474	-0.01368
O	-1.20150	-0.70809	-1.18304
H	-1.01529	-1.64804	-1.08249
O	1.18308	0.53207	-1.30237
H	0.67564	0.03208	-1.95369
C	-1.30796	-0.76548	1.22764
H	-0.93279	-0.32818	2.15221
H	-2.39630	-0.70526	1.23663
H	-1.02448	-1.81787	1.20253
C	-1.39972	1.36079	-0.07711
H	-1.24896	1.90960	0.85082
H	-0.97492	1.93616	-0.89891
H	-2.47187	1.25589	-0.24021
C	1.41199	-1.32925	0.20645
H	2.48487	-1.25540	0.03173
H	1.25473	-1.67927	1.22558
H	1.00830	-2.07215	-0.48396
C	1.33953	1.03565	0.99687
H	1.01399	0.79121	2.00691
H	2.42901	0.99981	0.97278
H	1.02665	2.05136	0.76164

$(H_3C)_2$-COH-COH-$(CH_3)_2\cdots(H_2O)_3$
E(RM062X)=-616.82730473

O	-0.85880	1.82230	-0.08590

H	-1.55550	2.03850	0.54410
H	0.92030	2.13510	0.36740
O	1.86120	2.33820	0.51830
H	1.95800	2.34700	1.47620
H	2.84650	0.80190	0.13670
O	3.37560	-0.00480	-0.00650
H	3.85250	0.15170	-0.82770
H	2.32650	-1.51180	-0.34100
O	-0.92920	-1.85090	0.02870
O	1.82630	-2.32290	-0.54700
H	0.00320	-1.98780	-0.21620
H	2.08680	-2.95480	0.13040
C	-1.06230	-0.53470	0.57520
C	-1.07770	0.49540	-0.60200
C	0.06990	0.25980	-1.57410
H	-0.06420	-0.67990	-2.10610
H	0.08010	1.06840	-2.30480
H	1.03370	0.24180	-1.06850
C	-2.39750	0.47370	-1.36290
H	-2.31640	1.10390	-2.24840
H	-2.64330	-0.53960	-1.68060
H	-3.21330	0.85150	-0.74720
C	-2.37410	-0.53510	1.34960
H	-2.27380	-1.17760	2.22430
H	-2.63360	0.46670	1.69510
H	-3.19100	-0.91300	0.73730
C	0.08750	-0.26890	1.54440
H	-0.06230	0.66620	2.08230
H	0.12230	-1.08140	2.27040
H	1.04770	-0.22340	1.03370

$(H_3C)_2$-COH-COH-$(CH_3)_2\cdots(H_2O)_4$

E(RM062X)=-693.272070878

O	1.27050	-1.75710	-0.46920
H	2.10650	-2.02460	-0.07210
H	-0.28780	-2.58080	-0.07410
O	-1.13130	-3.02680	0.12750
H	-1.40870	-3.42650	-0.70290
H	-2.36060	-1.77250	0.53590
O	-3.08190	-1.15380	0.76580
H	-2.83330	-0.79510	1.62380
H	-3.01520	0.31220	-0.29100
O	-3.06730	1.13420	-0.81750
H	-2.72520	0.89530	-1.68510
H	-1.81740	2.33180	-0.28640
O	1.33230	1.81280	0.45980
O	-1.15550	3.01780	-0.07240
H	0.45030	2.15550	0.23030
H	-1.39400	3.32980	0.80610

C	1.24920	0.40360	0.68840
C	1.28210	-0.33450	-0.69090
C	0.02810	-0.05410	-1.50690
H	-0.11800	1.01800	-1.63920
H	0.12680	-0.51100	-2.49160
H	-0.85430	-0.47090	-1.02170
C	2.52430	0.02000	-1.49870
H	3.43330	-0.28750	-0.98200
H	2.48530	-0.49880	-2.45620
H	2.57590	1.09060	-1.68680
C	2.45960	0.04850	1.54340
H	2.37650	0.56030	2.50180
H	2.51010	-1.02220	1.74110
H	3.38730	0.36440	1.06910
C	-0.03120	0.09190	1.45750
H	-0.15470	-0.98180	1.59910
H	0.01730	0.56600	2.43820
H	-0.90710	0.47750	0.93560

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