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Intramoleculer Hydrogen Bonding In Epoxide, Thiirane, Aziridine And Phosphirane Containing Cyclopentanols

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INTRAMOLECULER HYDROGEN BONDING IN EPOXIDE, THIIRANE, AZIRIDINE AND PHOSPHIRANE CONTAINING CYCLOPENTANOLS

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ABSTRACT

A recent computational analysis of the stabilizing intramolecular OH$\cdots$O contact in 1,2-dialkyl-2,3-epoxycyclopentanol diastereomers has been extended to thiiriane, aziridine and phosphirane analogues. Density functional theory (DFT), second-order Møller-Plesset perturbation theory (MP2) and CCSD(T) coupled-cluster computations with simple methyl and ethyl substituents indicate that electronic energies of the *cis* isomers are lowered by roughly 3 to 4 kcal mol^{-1} when the OH group of these cyclopentanol systems forms an intramolecular contact with the O, S, N or P atom on the adjacent carbon. The results also suggest that S and P can participate in these stabilizing intramolecular interactions as effectively as O and N in constrained molecular environments. The stabilizing intramolecular OH$\cdots$O, OH$\cdots$S, OH$\cdots$N and OH$\cdots$P contacts also increase the covalent OH bond length and significantly decrease the OH stretching vibrational frequency in every system with shifts typically on the order of -41 cm^{-1}.

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CHAPTER 1

INTRODUCTION

Previously known as the epoxy alcohol-aldol rearrangement[2], the Type III semipinacol rearrangement reaction[3,4] is the Lewis acid-mediated conversion of 2,3-epoxyalcohols to the corresponding β-hydroxycarbonyl (Figure 1.1). This conversion, which can be accomplished with a wide range of Lewis acids[5–10], is often accompanied by 1,2-alkyl migration, a transformation that is historically regarded as a convenient route to accessing chiral quaternary centers. Apart from its presence in numerous synthetic methodologies, the reactions appeal is evident in industrial and commercial applications[11] as well as in the preparation of a variety of natural products[12–15]. Despite its utility, however, the mechanistic details of the semipinacol rearrangement are poorly understood. Chemists generally agree that an antiperiplanar arrangement between the migrating group (M in Figure 1.1) and the adjacent, epoxide CO bond is necessary to drive the reaction[11,16], an arrangement that explains why *trans* diastereomers fail to react[8,17]. However, additional, proposed mechanistic details for Type III semipinacol rearrangements[18–21] are not supported by experimental or theoretical evidence. This apparent void sparked an initial interest in investigating why 2,3-epoxyalcohols rearrange to the corresponding ketols.

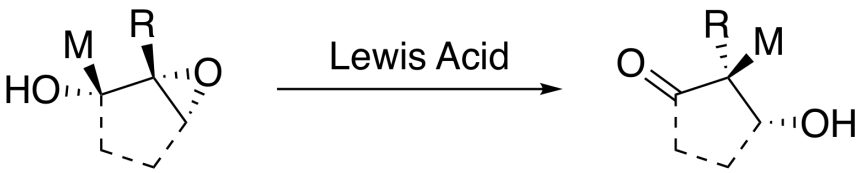

Figure 1.1. Lewis Acid-mediated Type III semipinacol rearrangement reaction converts 2,3-epoxyalcohols into the corresponding 1,3-ketol with concurrent 1,2-M group migration

To gain insight into these reactions, we recently examined the *cis/trans* energy differences in simple 1,2-dialkyl-2,3-epoxycyclopentanols[22]. Our quantum mechanical electronic structure computations from that study indicated that the *trans* diastereomers (right panel in Figure 1.2) had lower electronic energies than the corresponding *cis* structures in which the OH group pointed away from the epoxide (left panel in Figure 1.2). The corresponding relative energy is denoted $E_{rel}^{-h.b.}$ and depicted schematically in the top half of Figure 1.3. However, when the OH group was rotated toward the epoxide O atom in the *cis* diastereomers (center panel in Figure 1.2), the substrate exhibited significant stabilization, yielding electronic energies lower than those of the *trans* structures. This relative energy is labeled $E_{rel}^{+h.b.}$ and illustrated in the bottom half of Figure 1.3. To our knowledge, the OH$\cdots$O interaction identified in that study was the first instance of a stabilizing intramolecular contact between epoxide and alcohol moieties to be reported. Furthermore, those findings offered compelling evidence indicating that intramolecular proton transfer may be involved in the mechanism responsible for converting the 1,2-dialkyl-2,3-epoxyalcohol to the corresponding 2,2-dialkyl-1,3-ketol.

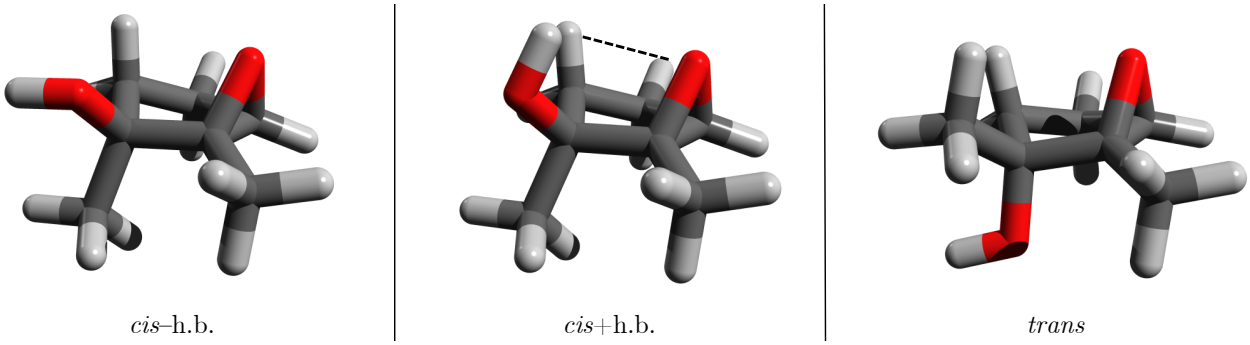

Figure 1.2. Three structural motifs of the 1,2-dimethyl-2,3-epoxycyclopentanols examined in Ref. 4: *cis* isomer without hydrogen bond (left), *cis* isomer with hydrogen bond (center), *trans* isomer (right).

The present study seeks to further characterize this intramolecular contact and any potential effects on the *cis/trans* energy differences of the aziridine, phosphirane and thi-

irane analogs of 1,2-dialkyl-2,3-epoxycyclopentanol. Specifically, our goal is to quantify any relative energy changes resulting from an intramolecular OH$\cdots$N, OH$\cdots$P or OH$\cdots$S contact because N, P and S atoms can also potentially act as hydrogen bond acceptors. An extensive literature search revealed some stabilization in molecules containing alcohol and aziridine functional groups through an OH$\cdots$N contact[23–28]. Because this interaction was similar to the OH$\cdots$O contact reported in Reference[22], we anticipated that 1,2-dialkyl-2,3-aziridinylcyclopentanol would also adopt three comparable arrangements as shown in Figure 1.4. No instances of corresponding intramolecular OH$\cdots$P or OH$\cdots$S stabilizing contacts for phosphirane- and thiirane-containing systems have been reported, but the capacity of P and S atoms to accept intramolecular hydrogen bonds is well established both experimentally and theoretically[26,29–34].

This investigation also provides some important theoretical extensions to the analysis presented in Reference[22]. In this work, the electronic structure computations are expanded to probe the effects of adding diffuse functions to the atomic orbital Gaussian basis sets. More

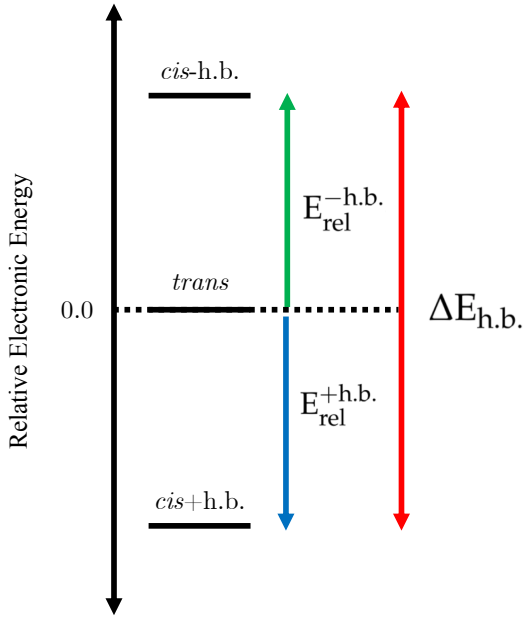

Figure 1.3. A schematic of the relative energies of the three different structural motifs: *cis* isomer without hydrogen bond, *cis* isomer with hydrogen bond, *trans* isomer.

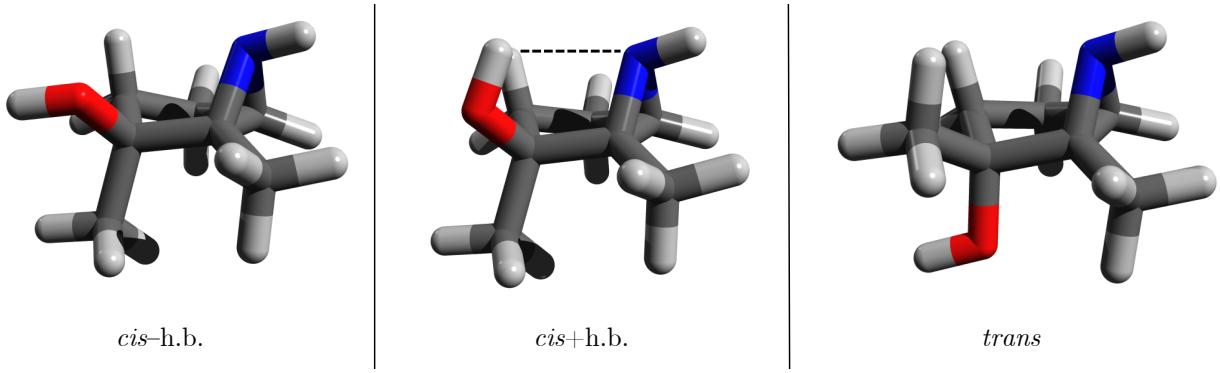

Figure 1.4. Three structural motifs of the 1,2-dimethyl-2,3-aziridine cyclopentanols: *cis* isomer without hydrogen bond (left), *cis* isomer with hydrogen bond (center), *trans* isomer (right).

importantly, quantification of these intramolecular contacts is extended beyond a simple relative energy scheme, which can overestimate the strength of the interaction[35], in contrast to intermolecular hydrogen bonds where direct computation of the hydrogen bond strength is relatively straightforward[36–39]. Thus, this investigation also reports physical characteristics, such as changes in OH stretching frequencies and other metrics widely considered among chemists to be distinctive features of hydrogen bonding.

In this paper, the term "hydrogen bond" is utilized to describe all reported OH$\cdots$A contacts, where A = O, S, N and P. This semantic decision is predicated on the well-established role that intramolecular hydrogen bonding plays in conformer stabilization[40–48]. Although the "qualifying features of a hydrogen bond are contentious" [49], particularly in constrained intramolecular environments such as between functional groups located on adjacent carbon atoms, there is strong experimental and theoretical evidence supporting intramolecular hydrogen bonding in instances that do not fit the formal definition[35,49–51]. Ultimately, this designation has no impact on the results presented in this manuscript. It merely simplifies the discussion of the relative energetics of the various *cis* and *trans* structures.

CHAPTER 2

COMPUTATIONAL METHODS

To probe the ability of the thiirane, aziridine and phosphirane groups to accept an intramolecular hydrogen bond in the same manner as the epoxide group in the 1,2-dialkyl-2,3-epoxycyclopentanol systems, this work employs methyl (Me) and ethyl (Et) alky substituents in three different substitution patterns at the M/R positions (Figure 1.1): Me/Me, Me/Et and Et/Me. For these twelve different systems, the following three distinct configurations are examined: *trans* configuration; *cis* configuration with the intramolecular hydrogen bond (*cis*+h.b.); *cis* configuration without the intramolecular hydrogen bond (*cis*−h.b.). These variations give a total of 36 unique structures examined in this study, 6 of which are shown in Figures 1.2 and 1.4.

Full geometry optimizations were performed on all 36 structures with the M06-2X[52] global hybrid density functional theory (DFT) method and two sets of correlation consistent triple zeta basis sets, one without and one with diffuse functions on all atoms (cc-pVTZ[53] and aug-cc-pVTZ[54,55] simply denoted TZ and aTZ ,respectively, hereafter). M06-2X harmonic vibrational frequencies were also computed with the TZ and aTZ basis sets for every optimized structure to ensure they are minima with no imaginary frequencies ($n_i = 0$). For systems containing S and P, M06-2X computations were also performed using the cc-pV(T+*d*)Z basis set[56] for those centers and the TZ basis set for all other atoms, but those results have been relegated to the Appendix because they are virtually identical to the M06-2X/TZ data discussed in detail in the next section. The nuclear magnetic resonance (NMR) chemical shielding constants were also calculated[57] at the M06-2X/TZ level of theory using the gauge-independent atomic orbital (GIAO) method[58].

Although prior studies[59,60] have shown the M06-2X functional can provide reliable conformational energetics for systems exhibiting intramolecular hydrogen bonding, MP2[61] geometry optimizations and harmonic vibrational frequency computations were also carried out in this work with the same TZ basis set to provide an additional estimate of the energetics associated with these inter and intramolecular interactions. Using the MP2/TZ geometries, a subsequent set of single point energy computations were carried out with the CCSD(T) coupled-cluster method that includes all single and double substitutions along with a perturbative estimate of connected triple excitations.

To examine the intrinsic energetics of these intramolecular contacts, all computations were carried out on the isolated molecular species. The M06-2X and MP2 computations were performed with the Gaussian 09 software package[62]. All structures were optimized without constraints, and the M06-2X computations employed the default numerical integration grid in Gaussian 09. The residual Cartesian forces of the optimized structures did not exceed 2.0×10^{-5} E_{h} a.u.$^{-1}$. The CCSD(T) energies were computed with Molpro 2015.[63,64] The *1s*-like core orbitals of C, N and O and the *1s*, *2s* and *2p*-like core orbitals of P and S were frozen during all MP2 and CCSD(T) computations.

It should be noted that NH$\cdots$O and PH$\cdots$O contacts were also examined in the *cis* configurations of the aziridine and phosphirane systems. Preliminary M06-2X computations, however, indicate that the structures in which the hydroxyl group accepts what could be described as an intramolecular hydrogen bond from NH or PH are not stabilized to the extent of the corresponding conformations in which the OH group acts as the hydrogen bond donor. As such, only results associated with the OH$\cdots$A interactions are reported and discussed here.

CHAPTER 3

RESULTS AND DISCUSSION

3.0.1 Energetics

In this study, the proposed stabilizing effects of the intramolecular OH$\cdots$O, OH$\cdots$S, OH$\cdots$N and OH$\cdots$P interactions were investigated in a series of 1,2-dialkyl-2,3-epoxy, thiiranyl, aziridinyl and phosphiranyl cyclopentanols. Because the *cis/trans* energetics appear to play such an important role in the underlying chemistry of Type III semipinacol rearrangement reactions, the same relative energies utilized in Reference[22] have been adopted for the current study ($E_{rel}^{+h.b.}$, $E_{rel}^{-h.b.}$ and $\Delta E_{h.b.}$). These terms are explicitly defined in Equations 1-3 and depicted schematically in Figure 1.3.

$$E_{rel}^{-h.b.} = E_{cis-h.b.} - E_{trans} \qquad \text{(Eq. 1)}$$

$$E_{rel}^{+h.b.} = E_{cis+h.b.} - E_{trans} \qquad \text{(Eq. 2)}$$

$$\Delta E_{h.b.} = E_{cis-h.b.} - E_{cis+h.b.} = E_{rel}^{-h.b.} - E_{rel}^{+h.b.} \qquad \text{(Eq. 3)}$$

The relative *cis/trans* electronic energies of the isolated (*in vacuo*) species are reported in Table 3.1 for the TZ basis set. (The data for other basis sets is available in the Appendix.) All 3 methods give remarkably consistent results, and they indicate that the electronic energy of the *trans* configuration are significantly lower than those of the non-hydrogen bonded *cis* diastereomers. The corresponding M06-2X, MP2 and CCSD(T) $E_{rel}^{-h.b.}$ values (Equation 1) range from +2.0 to +3.6 kcal mol^{-1} for these systems. The identity of the bridging heteroatom (A) only has modest effect on these *cis/trans* energy differences, increasing $E_{rel}^{-h.b.}$ by approximately 0.8 kcal mol^{-1} from the smallest values (for A = P and O) to the largest

(for A = N). Replacing the Me group with Et at either the M or R position has a similar effect and can increase $E_{rel}^{-h.b.}$ by roughly same amount: from +2.2 to +2.9 kcal mol^{-1} in the epoxide substrates (A = O), from +2.5 to +3.3 kcal mol^{-1} in the thiirane systems (A = S), from +2.8 to +3.6 kcal mol^{-1} in the aziridine compounds (A = N) and from +2.0 to +2.9 kcal mol^{-1} in the phosphirane analogs (A = P).

Table 3.1. Relative electronic energies ($E_{rel}^{-h.b.}$, $E_{rel}^{+h.b.}$, $\Delta E_{h.b.}$all in kcal mol^{-1}) computed with the TZ basis set.

A	M	R	M06-2X			MP2			CCSD(T)//MP2		
			$E_{rel}^{-h.b.}$	$E_{rel}^{+h.b.}$	$\Delta E_{h.b.}$	$E_{rel}^{-h.b.}$	$E_{rel}^{+h.b.}$	$\Delta E_{h.b.}$	$E_{rel}^{-h.b.}$	$E_{rel}^{+h.b.}$	$\Delta E_{h.b.}$
O	Me	Me	+2.2	−0.6	−2.8	+2.2	−0.6	−2.7	+2.2	−0.5	−2.8
O	Et	Me	+2.8	−0.7	−3.5	+2.7	−0.6	−3.2	+2.7	−0.4	−3.1
O	Me	Et	+2.6	−0.5	−3.1	+2.8	−0.3	−3.1	+2.9	−0.2	−3.1
S	Me	Me	+2.5	−0.8	−3.3	+2.6	−0.8	−3.3	+2.6	−0.7	−3.3
S	Et	Me	+3.3	−0.6	−3.9	+3.3	−0.4	−3.7	+3.3	−0.1	−3.4
S	Me	Et	+2.9	−0.6	−3.6	+3.4	−0.3	−3.6	+3.4	−0.2	−3.2
N	Me	Me	+2.8	−0.9	−3.7	+2.8	−0.9	−3.6	+2.8	−0.9	−3.7
N	Et	Me	+3.5	−0.4	−3.9	+3.5	−0.4	−3.9	+3.4	−0.5	−3.9
N	Me	Et	+3.2	−0.8	−4.1	+3.6	−0.6	−4.1	+3.5	−0.6	−4.1
P	Me	Me	+2.0	−0.5	−2.5	+2.2	−0.5	−2.7	+2.1	−0.4	−2.5
P	Et	Me	+2.9	−0.0	−2.9	+2.9	+0.1	−2.8	+2.4	−0.0	−2.4
P	Me	Et	+2.4	−0.3	−2.7	+2.8	−0.2	−3.0	+2.7	−0.1	−2.7

The M06-2X, MP2 and CCSD(T) $E_{rel}^{+h.b.}$ data provided in Table 3.1 and defined in Equation 2 show that all but one of the *cis* isomers become lower in energy than their *trans* counterparts when the OH group is oriented in the *cis* configuration to donate a hydrogen bond to the O, S, N or P atom. For the Me and Et substituted 1,2-dialkyl-2,3-epoxycyclopentanols, the *cis*+h.b. structures have lower electronic energies with the TZ basis set than the *trans* isomers by −0.2 to −0.7 kcal mol^{-1} when A = O. The $E_{rel}^{+h.b.}$ values are quite similar for A = S (−0.1 to −0.8 kcal mol^{-1}) and for A = N (−0.4 to −0.9 kcal mol^{-1}). Although the trend holds in the phosphirane systems, the *trans* and *cis*+h.b. systems become isoenergetic when the Et substituent is at position 1 (i.e., M = Et). Diffuse functions have a negligible impact on the M06-2X energetics reported in Table 3.1. The

corresponding results obtained with the aTZ basis set can be found in the Appendix.

The aforementioned relative energies provide insight into the magnitude of stabilization imparted by the intramolecular OH$\cdots$A contacts in these systems as defined by $\Delta E_{h.b.}$ in Equation 3. The M06-2X, MP2 and CCSD(T) values for the Me and Et substituted 1,2-dialkyl-2,3-epoxycyclopentanols range from -2.7 to -3.5 kcal mol^{-1} for the OH$\cdots$O interactions. The $\Delta E_{h.b.}$ values reported in Table 3.1 reveal that both the OH$\cdots$S and OH$\cdots$N intramolecular contacts in the systems examined here are potentially stronger, ranging from -3.3 to -3.9 kcal mol^{-1} for the former and -3.6 to -4.1 kcal mol^{-1} for the latter. Although slightly smaller in magnitude than the $\Delta E_{h.b.}$ values for the analogous OH$\cdots$O contacts, these estimates of the stabilization from the intramolecular OH$\cdots$P interaction still approach -3 kcal mol^{-1}.

The $\Delta E_{h.b.}$ values reported in Table 3.1 are entirely consistent with those published elsewhere for intramolecular vicinal hydrogen bonds with an OH donor. For example, an analogous computational analysis of 2-substituted ethanols (with fluoro, amino and nitro groups) yielded corresponding energy differences near 2 kcal mol^{-1} [50]. The *cis/trans* energy difference for 2-fluoro and 2-chlorophenol were found to be slightly larger and on the order of 3 or 4 kcal mol^{-1} from DFT and MP2 computations[51], which is perhaps not surprising given that phenols are significantly more acidic than cyclopentanols. Subsequent analyses of these constrained intramolecular contacts based on the electron density, orbitals and/or electrostatic potential[65–74] are avoided in the present study because they have been shown to yield rather inconsistent results[35,49].

3.0.2 Bond Lengths, Vibrational Frequencies and NMR Chemical Shielding Constants

When a hydroxyl group forms a typical intermolecular hydrogen bond, the vibrational frequency associated with the covalent OH bond stretch shifts to a lower energy (commonly referred to as a "red shift"). In the gas phase, for example, when one water molecule donates a hydrogen bond to another to form the water dimer, the donor OH stretching

frequency shifts to 3602 cm^{-1} which is 55 cm^{-1} lower than the symmetric OH stretch of the water monomer and 154 cm^{-1} lower than the asymmetric stretch[75,76]. Similar changes in spectroscopic and geometrical parameters are known to accompany intramolecular hydrogen bond formation[71–74,77,78].

Table 3.2 reports the analogous gas phase OH harmonic stretching frequencies computed with the M06-2X functional and the TZ basis set for all 36 optimized structures. The first three columns list the OH stretching frequencies for the *trans*, *cis*−h.b. and *cis*+h.b. systems, respectively. Although the OH groups adopt significantly different orientations in the *trans* and *cis*−h.b. configurations, the corresponding harmonic vibrational frequencies never differ by more than 5 cm^{-1} with the *cis*−h.b. frequency typically having a slightly larger value by +2 cm^{-1}. These differences are tabulated in the penultimate column of data denoted $\Delta\omega_{-\text{h.b.}}$ and are defined just like the energy difference in Equation 1.

Table 3.2. Absolute and relative M06-2X/TZ harmonic OH stretching frequencies (ω and $\Delta\omega$ in cm^{-1}).

A	M	R	ω_{trans}	$\omega_{-\text{h.b.}}$	$\omega_{+\text{h.b.}}$	$\Delta\omega_{-\text{h.b.}}$	$\Delta\omega_{+\text{h.b.}}$
O	Me	Me	3874	3872	3843	−2	−31
O	Et	Me	3880	3881	3841	+1	−40
O	Me	Et	3870	3872	3843	+2	−27
S	Me	Me	3873	3874	3830	+1	−42
S	Et	Me	3878	3882	3827	+4	−51
S	Me	Et	3869	3874	3828	+5	−41
N	Me	Me	3877	3874	3831	−3	−45
N	Et	Me	3883	3884	3832	+1	−50
N	Me	Et	3867	3873	3826	+1	−45
P	Me	Me	3871	3871	3837	−0	−34
P	Et	Me	3877	3878	3836	+1	−41
P	Me	Et	3868	3872	3836	+4	−32

In stark contrast, the OH stretching frequency is significantly perturbed in the *cis*+h.b. structures all of which exhibit the intramolecular OH$\cdots$A contacts. The last column of data in Table 3.2 gives the OH stretching frequency difference between the *trans* and *cis*+h.b. structures (analogous to the energy difference in Equation 2). The intramolecular OH$\cdots$A

contacts cause the frequency to decrease by at least 25 cm^{-1} and by as much as 51 cm^{-1} (with an average change of 41 cm^{-1}). The same trends are observed in the M06-2X/aTZ and MP2/TZ harmonic frequency computations within the Appendix. As with the conformational energy differences, the OH stretching frequency shifts reported here are consistent with the other computational studies of 2-substituted alcohols (e.g., -36 cm^{-1} for 2-fluoroethanol and -60 cm^{-1} for 2-nitroethanol)[50,79]. The shifts can be larger for less constrained intramolecular OH$\cdots$A contacts. The experimental difference between the free and hydrogen bonded OH stretches of 1,3-propanediol is -76 cm^{-1} [43], but that is still appreciably smaller than the corresponding -103 cm^{-1} shift induced by the formation of the analogous intermolecular hydrogen bond between methanol and dimethylether[32].

Table 3.3. Absolute and relative M06-2X/TZ covalent OH bond lengths (R and ΔR in Å).

A	M	R	R_{trans}	$R_{-h.b.}$	$R_{+h.b.}$	$\Delta R_{-h.b.}$	$\Delta R_{+h.b.}$
O	Me	Me	0.9609	0.9605	0.9633	−0.0004	+0.0024
O	Et	Me	0.9606	0.9605	0.9636	−0.0001	+0.0030
O	Me	Et	0.9612	0.9610	0.9635	−0.0002	+0.0022
S	Me	Me	0.9611	0.9610	0.9640	−0.0001	+0.0030
S	Et	Me	0.9607	0.9605	0.9641	−0.0002	+0.0034
S	Me	Et	0.9613	0.9610	0.9641	−0.0003	+0.0029
N	Me	Me	0.9608	0.9609	0.9642	+0.0001	+0.0034
N	Et	Me	0.9604	0.9602	0.9641	−0.0002	+0.0037
N	Me	Et	0.9611	0.9609	0.9644	−0.0001	+0.0034
P	Me	Me	0.9612	0.9611	0.9633	−0.0000	+0.0021
P	Et	Me	0.9608	0.9607	0.9633	−0.0001	+0.0024
P	Me	Et	0.9614	0.9611	0.9634	−0.0003	+0.0020

Table 3.3 provides the related geometrical parameters for each gas phase optimized structure. As expected, the trends in the covalent OH bond lengths reported in the first 3 columns of data are congruent with those for the OH stretching frequencies. The OH bond lengths are nearly identical for the corresponding *trans* and *cis*−h.b. structures. They never differ by more than 0.0004 Å ($\Delta R_{-h.b.}$), and the *cis*−h.b. bond length is almost always slightly shorter by approximately 0.0002 Å. In contrast, the differences in the bond lengths are an order of magnitude larger when comparing values for the *trans* and *cis*+h.b.

structures ($\Delta R_{+h.b.}$). The OH bond lengths in Table 3.3 are typically 0.003 Å longer in the structures exhibiting the intramolecular OH$\cdots$A contacts in accord with the appreciably lower OH stretching frequencies in Table 3.2. The same bond length changes can be seen for the M06-2X/aTZ and MP2/TZ data in the Appendix.

Table 3.4. Absolute and relative M06-2X/TZ isotropic NMR chemical shielding constants for the hydroxyl H atom (σ and $\Delta\sigma$ in ppm.)

A	M	R	σ_{trans}	$\sigma_{-h.b.}$	$\sigma_{+h.b.}$	$\Delta\sigma_{-h.b.}$	$\Delta\sigma_{+h.b.}$
O	Me	Me	31.90	31.42	31.01	−0.48	−0.90
O	Et	Me	31.12	30.86	30.72	−0.26	−0.40
O	Me	Et	31.89	31.47	30.88	−0.42	−1.01
S	Me	Me	31.84	31.35	30.84	−0.49	−1.00
S	Et	Me	31.14	30.62	30.71	−0.52	−0.43
S	Me	Et	31.80	31.34	30.72	−0.46	−1.08
N	Me	Me	31.90	31.51	30.57	−0.39	−1.32
N	Et	Me	31.22	30.90	30.54	−0.32	−0.68
N	Me	Et	31.96	31.59	30.40	−0.37	−1.56
P	Me	Me	31.96	31.42	31.11	−0.54	−0.86
P	Et	Me	31.27	30.62	31.12	−0.65	−0.15
P	Me	Et	31.94	31.49	31.01	−0.45	−0.94

The corresponding gas phase M06-2X/TZ isotropic NMR chemical shielding constants (σ) for the H atom in the OH functional groups are reported in the first 3 columns of data in Table 3.4 for the *trans*, *cis*−h.b. and *cis*+h.b. systems, respectively. The isotropic shielding constants range from 30.40 to 31.96 ppm with the *trans* isomers consistently giving the largest σ values. Without exception, the isotropic shielding constants for the *cis*−h.b. are smaller by −0.26 to −0.65 ppm as indicated by the $\Delta\sigma_{-h.b.}$ column of data. However, when the OH group rotates to form an OH$\cdots$A contact, σ tends to decrease further, by roughly a factor of 2, giving $\Delta\sigma_{+h.b.}$ values that grow to as much as −1.56 ppm (last column of Table 3.4). In other words, σ is generally smaller for the *cis*+h.b. structures and larger for the *cis*−h.b. conformations. The two exceptions to this trend occur when M = Et and A = S or P. Overall, both the sign and magnitude of these changes are consistent with the formation of intramolecular hydrogen bonds in similar systems.[72,73] The same trends are observed in

the M06-2X/aTZ and MP2/TZ NMR data reported in the Appendix. However, it should be noted that changes NMR chemical shifts (often denoted $\Delta\delta$) have the opposite sign as those associated with isotropic shielding constants ($\Delta\sigma$).

The properties discussed in this section, and changes thereof, are qualitatively consistent with hydrogen bond formation, and the Appendix includes graphs that explore these relationships by plotting the relative electronic energies of the *cis*+h.b. structures ($E_{rel}^{+h.b.}$ or $\Delta E_{h.b.}$) versus various metrics from Tables 3.2, 3.3 and 3.4. Only the $R_{+h.b.}$ and $\Delta R_{+h.b.}$ covalent OH bond length parameters in Table 3.3 have a clear correlation with $E_{rel}^{+h.b.}$ or $\Delta E_{h.b.}$, for which the coefficient of determination (r^2) from a simple linear regression ranges from 0.83 to 0.89. This value does not exceed 0.66 for any of the other relationships examined in the Appendix. Trends for certain subsets of data could emerge (e.g., for a given hydrogen bond acceptor) as additional systems are investigated, but no general relationships across all systems are apparent from the data plotted in the Appendix apart from those involving the covalent OH bond length. This result is perhaps not too surpising given the highly constrained nature of these intramolecular OH$\cdots$A contacts and the diversity of hydrogen bond accepts (A = O, S, N and P).

CHAPTER 4

CONCLUSIONS

The DFT, MP2 and CCSD(T) computations performed in this study reveal that all of the systems examined exhibit stabilizing OH$\cdots$A intramolecular interactions *in vacuo*, where A = O, S, N and P. A total of 36 unique structures were characterized to probe the relative *cis*/*trans* energetics with and without the intramolecular OH$\cdots$A interaction. With simple Me and Et substituents, the *cis* conformers electronic energies are stabilized by to 2.5 to 4.1 kcal mol^{-1} when the OH group rotates toward the adjacent O, S, N or P atoms. Consequently, the *cis* configurations exhibiting these intramolecular contacts have lower electronic energies than their *trans* counterparts. The intramolecular OH$\cdots$A contacts in the systems studied here also induce OH covalent bond elongation along with a commensurate decrease in the OH stretching frequency and the isotropic NMR chemical shielding constant for the hydroxyl H atom. These findings represent the first theoretical evidence describing a stabilizing intramolecular interaction between hydroxyl and thiirane/phosphirane moieties exhibiting many of the characteristics commonly associated intramolecular hydrogen bonding. From a synthetic perspective, the results also suggest that the *cis* diastereomers can potentially serve as a fascinating starting point toward accessing interesting β-keto alcohols, amines, thiols, and phosphines via Type III semipinacol rearrangement reaction. Future work will probe the distance and directional dependencies of these constrained intramolecular interactions in these cyclic and analogous acyclic systems.

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APPENDIX

Table S1: Optimized bond lengths and angles associated with the intramolecular OH···A contacts (R(H···A) in Å and θ(OH···A) in degrees, respectively).

			M06-2X/cc-pVTZ		M06-2X/aug-cc-pVTZ		MP2/cc-pVTZ	
A	M	R	R(H···A)	θ(OH···A)	R(H···A)	θ(OH···A)	R(H···A)	θ(OH···A)
O	Me	Me	2.59	104	2.61	103	2.53	105
O	Et	Me	2.50	106	2.50	106	2.47	108
O	Me	Et	2.54	105	2.54	105	2.53	107
S	Me	Me	2.78	112	2.79	111	2.76	113
S	Et	Me	2.70	114	2.70	113	2.65	116
S	Me	Et	2.72	113	2.73	112	2.69	115
NH	Me	Me	2.53	107	2.55	106	2.52	108
NH	Et	Me	2.51	108	2.46	108	2.50	109
NH	Me	Et	2.48	108	2.50	108	2.44	110
PH	Me	Me	2.83	113	2.83	113	2.80	115
PH	Et	Me	2.74	115	2.74	115	2.69	118
PH	Me	Et	2.79	114	2.79	114	2.74	116

Table S2: Absolute and relative M06-2X covalent OH bond lengths (R and ΔR in Å) computed with the cc-pV(T+d)Z basis set.

A	M	R	R_{trans}	$R_{-\text{h.b.}}$	$R_{+\text{h.b.}}$	$\Delta R_{-\text{h.b.}}$	$\Delta R_{+\text{h.b.}}$
S	Me	Me	0.96105	0.96099	0.96339	−0.0001	+0.0023
S	Et	Me	0.96070	0.96051	0.96405	−0.0002	+0.0033
S	Me	Et	0.96125	0.96097	0.96408	−0.0003	+0.0028
PH	Me	Me	0.96118	0.96113	0.96329	+0.0000	+0.0021
PH	Et	Me	0.96082	0.96071	0.96323	−0.0001	+0.0024
PH	Me	Et	0.96131	0.96108	0.96334	−0.0002	+0.0020

Table S3: Absolute and relative M06-2X harmonic OH stretching frequencies (ω and $\Delta\omega$ in cm^{-1}) computed with the cc-pV(T+d)Z basis set.

A	M	R	ω_{trans}	$\omega_{-\text{h.b.}}$	$\omega_{+\text{h.b.}}$	$\Delta\omega_{-\text{h.b.}}$	$\Delta\omega_{+\text{h.b.}}$
S	Me	Me	3874	3831	3873	−42	−43
S	Et	Me	3882	3828	3878	−50	−54
S	Me	Et	3874	3829	3869	−41	−45
PH	Me	Me	3871	3838	3871	−33	−33
PH	Et	Me	3878	3836	3877	−41	−42
PH	Me	Et	3871	3836	3868	−32	−35

Table S4: Absolute and relative M06-2X harmonic OH stretching frequencies (ω and $\Delta\omega$ in cm^{-1}) computed with the aTZ basis set.

A	M	R	ω_{trans}	$\omega_{-h.b.}$	$\omega_{+h.b.}$	$\Delta\omega_{-h.b.}$	$\Delta\omega_{+h.b.}$
O	Me	Me	3869	3872	3840	+3	−29
O	Et	Me	3875	3876	3838	+1	−38
O	Me	Et	3865	3868	3841	+3	−25
S	Me	Me	3868	3870	3825	+2	−43
S	Et	Me	3873	3876	3823	+3	−51
S	Me	Et	3870	3870	3824	−0	−46
N	Me	Me	3872	3870	3829	−2	−44
N	Et	Me	3874	3873	3823	−1	−52
N	Me	Et	3867	3867	2824	+0	−43
P	Me	Me	3867	3867	3833	+1	−33
P	Et	Me	3872	3875	3831	+3	−41
P	Me	Et	3862	3868	3831	+5	−31

Table S5: Absolute and relative M06-2X covalent OH bond lengths (R and ΔR in Å) computed with the aTZ basis set.

A	M	R	R_{trans}	$R_{-h.b.}$	$R_{+h.b.}$	$\Delta R_{-h.b.}$	$\Delta R_{+h.b.}$
O	Me	Me	0.96087	0.96086	0.96310	−0.0000	+0.0022
O	Et	Me	0.96052	0.96038	0.96337	−0.0001	+0.0028
O	Me	Et	0.96111	0.96088	0.96325	−0.0002	+0.0021
S	Me	Me	0.96099	0.96089	0.96395	−0.0001	+0.0030
S	Et	Me	0.96066	0.96040	0.96402	−0.0003	+0.0034
S	Me	Et	0.96093	0.96085	0.96405	−0.0001	+0.0031
NH	Me	Me	0.96070	0.96082	0.96398	+0.0001	+0.0033
NH	Et	Me	0.96057	0.96070	0.96428	+0.0001	+0.0037
NH	Me	Et	0.96095	0.96098	0.96419	−0.0000	+0.0032
PH	Me	Me	0.96110	0.96098	0.96324	−0.0001	+0.0021
PH	Et	Me	0.96076	0.96057	0.96320	−0.0002	+0.0024
PH	Me	Et	0.96129	0.96093	0.96329	−0.0004	+0.0020

Table S6: Absolute and relative MP2 covalent OH bond lengths (R and ΔR in Å) computed with the TZ basis set.

A	M	R	R_{trans}	$R_{-\text{h.b.}}$	$R_{+\text{h.b.}}$	$\Delta R_{-\text{h.b.}}$	$\Delta R_{+\text{h.b.}}$
O	Me	Me	0.9635	0.9633	0.9655	−0.0002	+0.0020
O	Et	Me	0.9631	0.9628	0.9661	−0.0004	+0.0030
O	Me	Et	0.9638	0.9634	0.9658	−0.0004	+0.0020
S	Me	Me	0.9639	0.9636	0.9667	−0.0003	+0.0029
S	Et	Me	0.9636	0.9631	0.9673	−0.0005	+0.0037
S	Me	Et	0.9639	0.9636	0.9671	−0.0003	+0.0031
NH	Me	Me	0.9635	0.9633	0.9666	−0.0001	+0.0032
NH	Et	Me	0.9631	0.9627	0.9668	−0.0004	+0.0037
NH	Me	Et	0.9639	0.9635	0.9671	−0.0004	+0.0033
PH	Me	Me	0.9641	0.9638	0.9663	−0.0003	+0.0022
PH	Et	Me	0.9637	0.9634	0.9668	−0.0003	+0.0031
PH	Me	Et	0.9646	0.9639	0.9666	−0.0007	+0.0020

Table S7: Absolute and relative MP2 harmonic OH stretching frequencies (ω and $\Delta\omega$ in cm^{-1}) computed with the TZ basis set.

A	M	R	ω_{trans}	$\omega_{-\text{h.b.}}$	$\omega_{+\text{h.b.}}$	$\Delta\omega_{-\text{h.b.}}$	$\Delta\omega_{+\text{h.b.}}$
O	Me	Me	3830	3801	3826	−26	−29
O	Et	Me	3838	3792	3832	−40	−46
O	Me	Et	3828	3796	3820	−24	−31
S	Me	Me	3826	3776	3821	−45	−50
S	Et	Me	3834	3764	3826	−62	−70
S	Me	Et	3824	3809	3814	−5	−15
NH	Me	Me	3859	3814	3862	−48	−45
NH	Et	Me	3870	3815	3868	−53	−55
NH	Me	Et	3859	3810	3856	−46	−48
PH	Me	Me	3857	3819	3856	−36	−37
PH	Et	Me	3864	3817	3861	−44	−47
PH	Me	Et	3857	3818	3851	−33	−39

Table S8: Absolute and relative M06-2X/aTZ isotropic NMR chemical shielding constants for the hydroxyl H atom (σ and $\Delta\sigma$ in ppm).

A	M	R	σ_{trans}	$\sigma_{-\text{h.b.}}$	$\sigma_{+\text{h.b.}}$	$\Delta\sigma_{-\text{h.b.}}$	$\Delta\sigma_{+\text{h.b.}}$
O	Me	Me	31.74	31.32	30.94	−0.42	−0.80
O	Et	Me	31.00	30.79	30.74	−0.21	−0.27
O	Me	Et	31.64	31.30	30.88	−0.34	−0.76
S	Me	Me	31.65	31.18	30.83	−0.46	−0.81
S	Et	Me	30.95	30.54	30.67	−0.41	−0.28
S	Me	Et	31.58	31.16	30.66	−0.42	−0.92
NH	Me	Me	31.91	30.57	30.64	−1.35	−1.27
NH	Et	Me	30.99	30.72	30.34	−0.27	−0.65
NH	Me	Et	31.74	31.32	30.44	−0.42	−1.30
PH	Me	Me	31.76	31.24	31.11	−0.52	−0.65
PH	Et	Me	31.07	30.50	30.95	−0.58	−0.12
PH	Me	Et	31.77	31.25	30.93	−0.53	−0.84

Table S9: Absolute and relative MP2/TZ isotropic NMR chemical shielding constants for the hydroxyl H atom (σ and $\Delta\sigma$ in ppm).

A	M	R	σ_{trans}	$\sigma_{-\text{h.b.}}$	$\sigma_{+\text{h.b.}}$	$\Delta\sigma_{-\text{h.b.}}$	$\Delta\sigma_{+\text{h.b.}}$
O	Me	Me	31.47	31.39	30.58	−0.08	−0.89
O	Et	Me	31.11	30.43	30.55	−0.68	−0.56
O	Me	Et	31.77	31.02	30.68	−0.74	−1.08
S	Me	Me	31.37	30.90	30.63	−0.47	−0.74
S	Et	Me	31.09	30.71	30.45	−0.39	−0.65
S	Me	Et	31.68	31.38	30.62	−0.30	−1.06
NH	Me	Me	31.87	31.09	30.48	−0.78	−1.39
NH	Et	Me	31.23	30.97	30.44	−0.26	−0.78
NH	Me	Et	31.88	31.54	30.25	−0.34	−1.63
PH	Me	Me	31.74	31.40	30.87	−0.34	−0.87
PH	Et	Me	31.28	30.32	30.90	−0.96	−0.38
PH	Me	Et	31.88	31.53	30.91	−0.34	−0.97

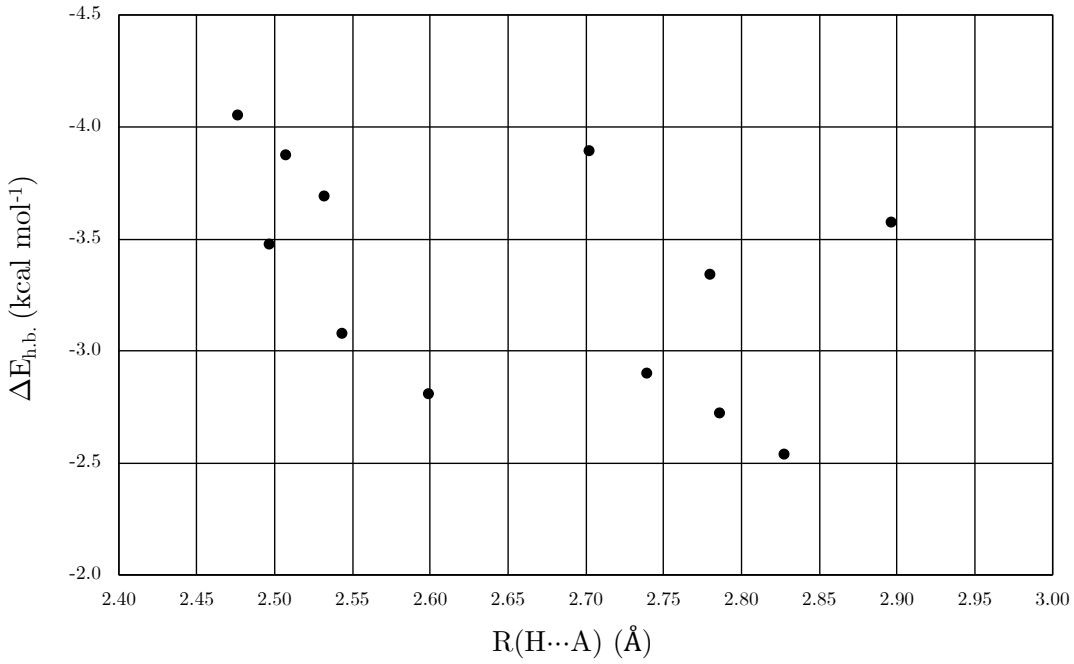

Figure S1: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($\Delta E_{h.b.}$ in kcal mol^{-1} as defined by Equation 3) versus the H$\cdots$A distances (R(H$\cdots$A) in Å) associated with the intramolecular hydrogen bonds. Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

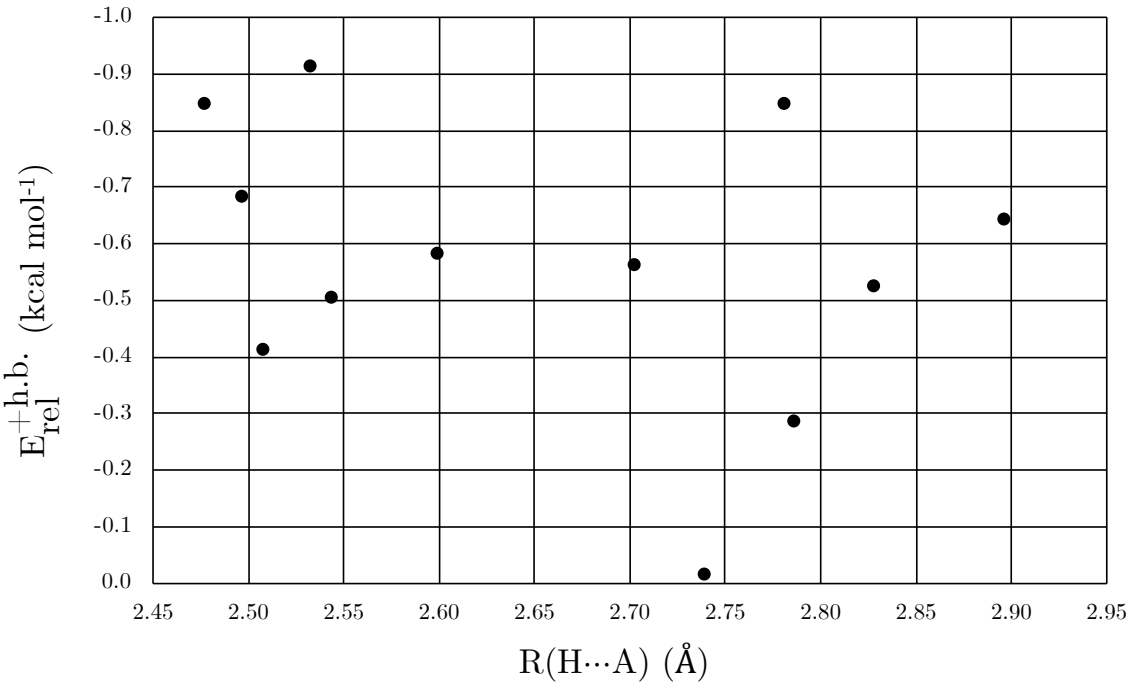

Figure S2: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($E_{rel}^{+h.b.}$ in kcal mol^{-1} as defined by Equation 2) versus the H$\cdots$A distances (R(H$\cdots$A) in Å) associated with the intramolecular hydrogen bonds. Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

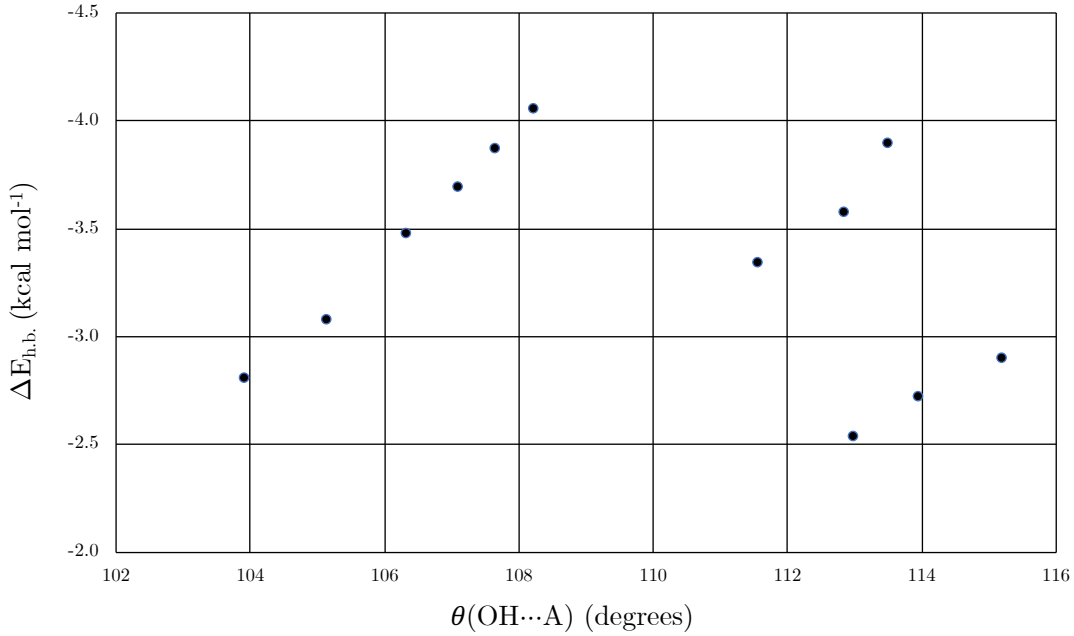

Figure S3: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($\Delta E_{h.b.}$ in kcal mol^{-1} as defined by Equation 3) versus the OH···A bond angles (θ(OH···A) in degrees) associated with the intramolecular hydrogen bonds. Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

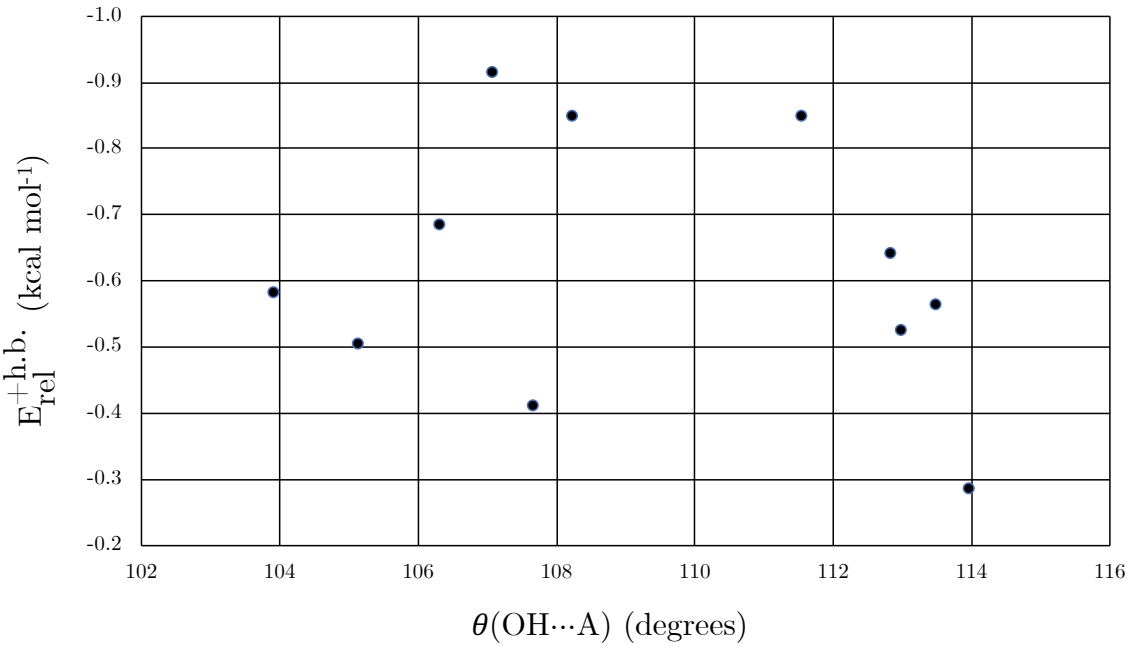

Figure S4: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($E_{rel}^{+h.b.}$ in kcal mol^{-1} as defined by Equation 2) versus the OH···A bond angles (θ(OH···A) in degrees) associated with the intramolecular hydrogen bonds. Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

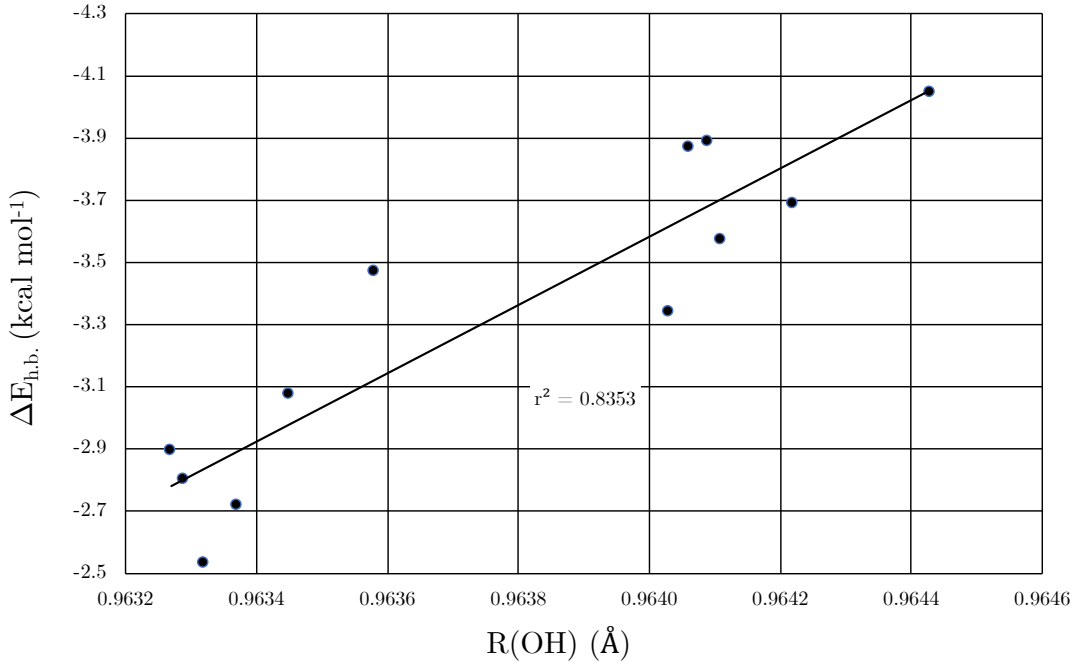

Figure S5: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($\Delta E_{h.b.}$ in kcal mol^{-1} as defined by Equation 3) versus the *cis*+h.b. covalent OH bond lengths (R(OH) in Å). Trend lines and coefficients of determination are shown when $r^2 > 0.5$.

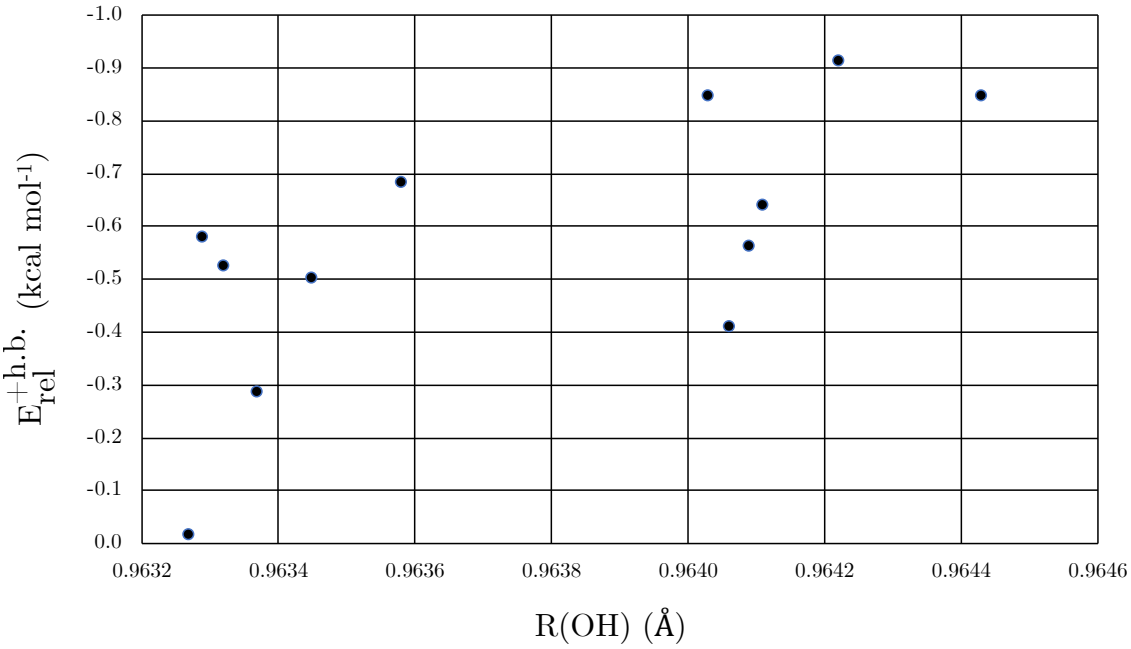

Figure S6: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($E_{rel}^{+h.b.}$ in kcal mol^{-1} as defined by Equation 2) versus the *cis*+h.b. covalent OH bond lengths (R(OH) in Å). Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

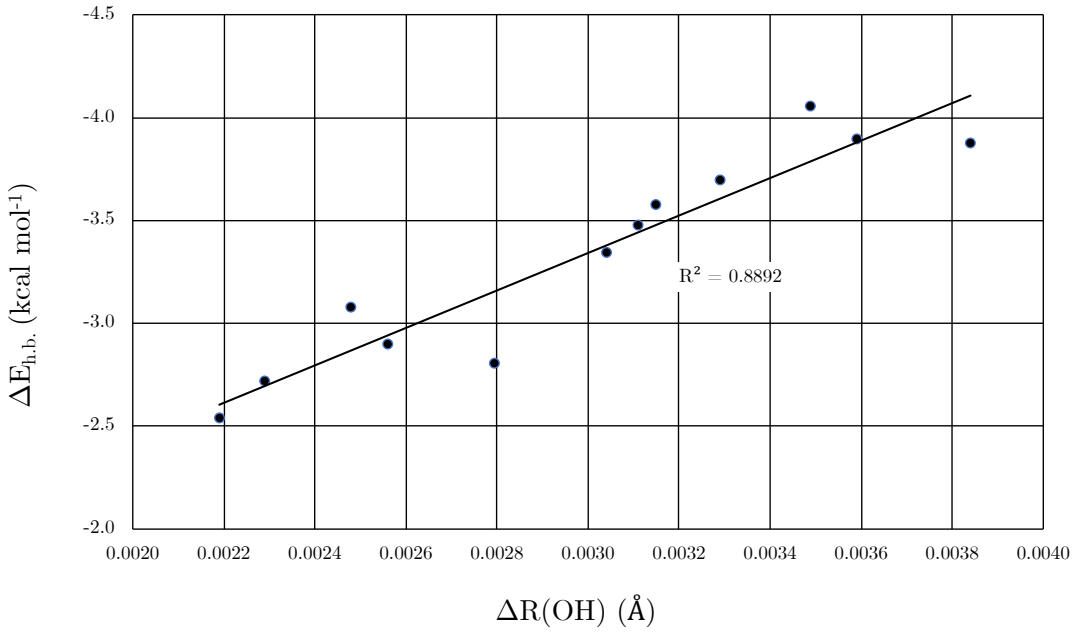

Figure S7: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($\Delta E_{h.b.}$ in kcal mol^{-1} as defined by Equation 3) versus the corresponding changes in the covalent OH bond lengths (ΔR(OH) in Å). Trend lines and coefficients of determination are shown when $r^2 > 0.5$.

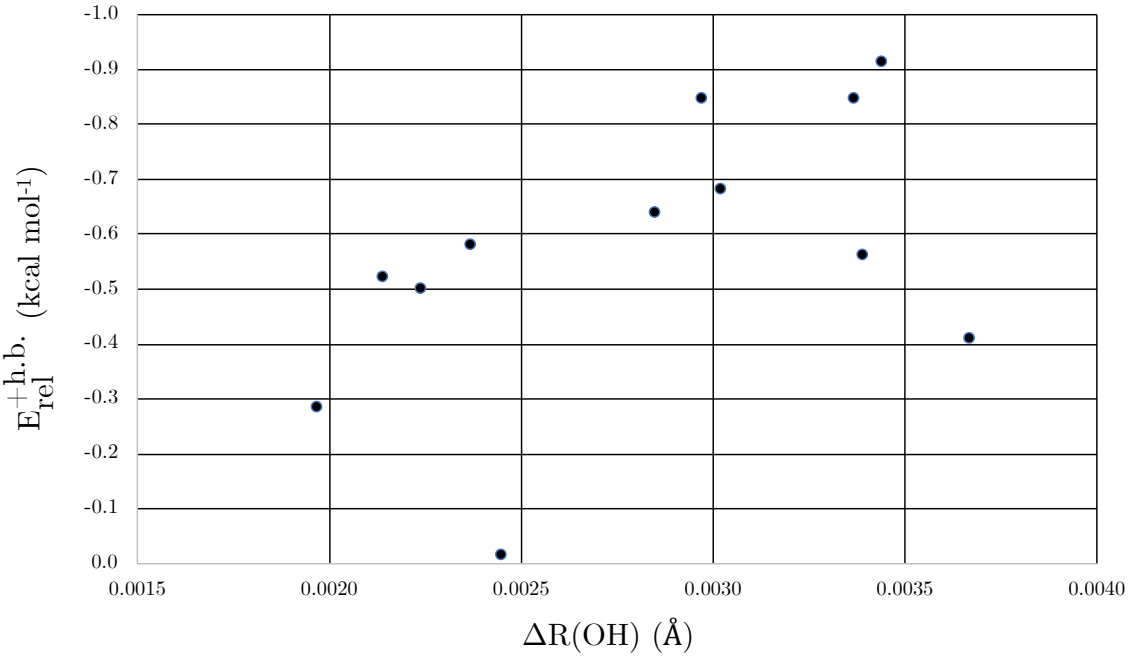

Figure S8: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($E_{rel}^{+h.b.}$ in kcal mol^{-1} as defined by Equation 2) versus the corresponding changes in the covalent OH bond lengths (ΔR(OH) in Å). Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

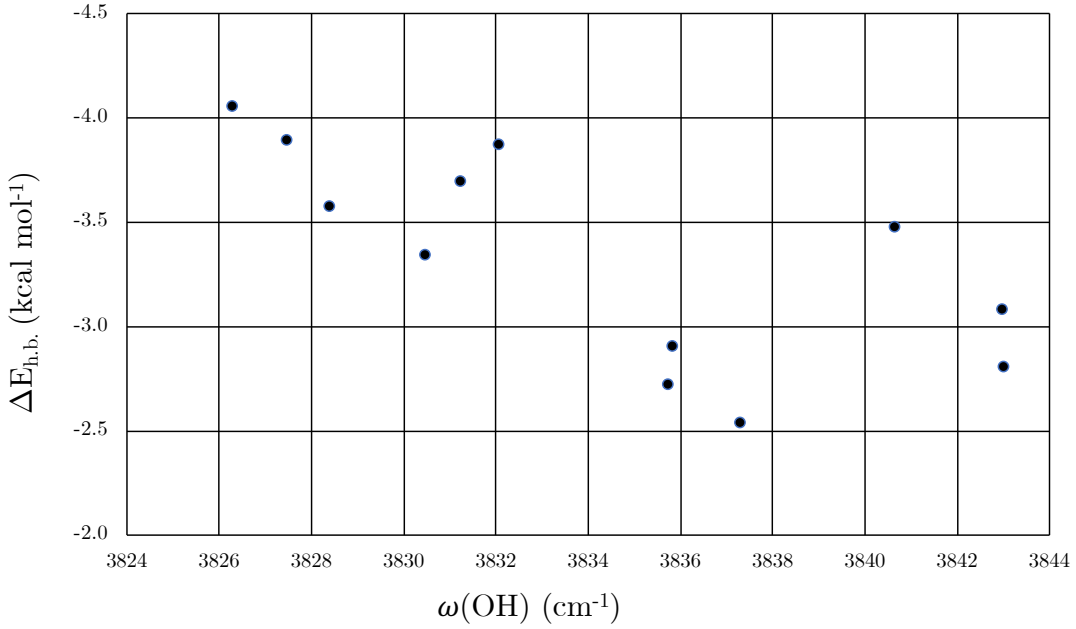

Figure S9: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($\Delta E_{h.b.}$ in kcal mol^{-1} as defined by Equation 3) versus the *cis*+h.b. harmonic OH stretching frequencies (ω(OH) in cm^{-1}). Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

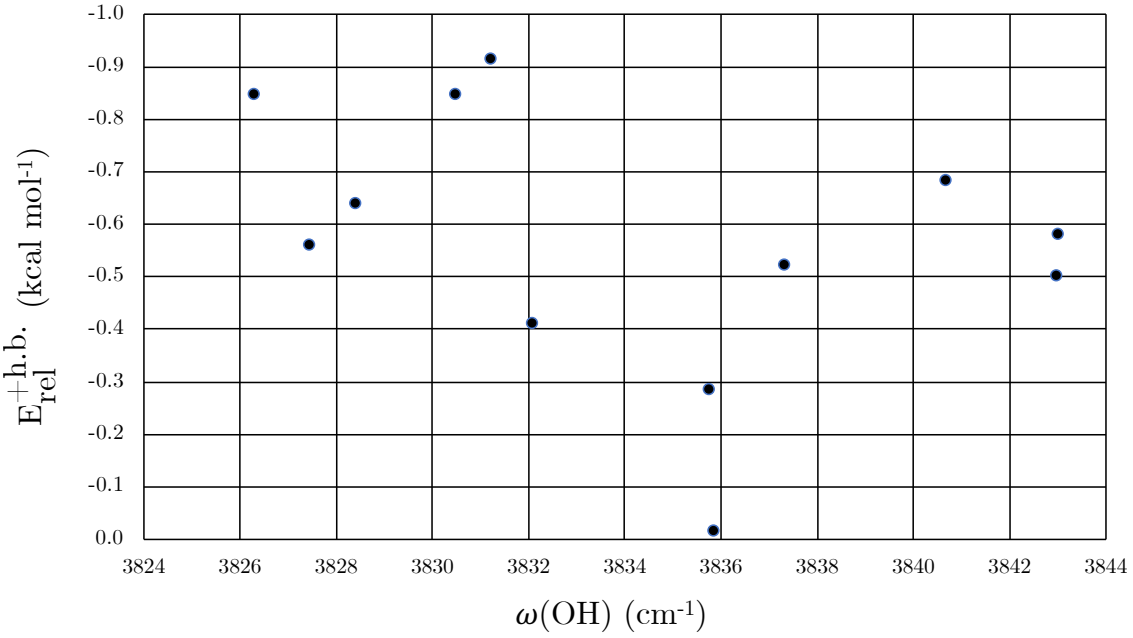

Figure S10: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($E_{rel}^{+h.b.}$ in kcal mol^{-1} as defined by Equation 2) versus the *cis*+h.b. harmonic OH stretching frequencies (ω(OH) in cm^{-1}). Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

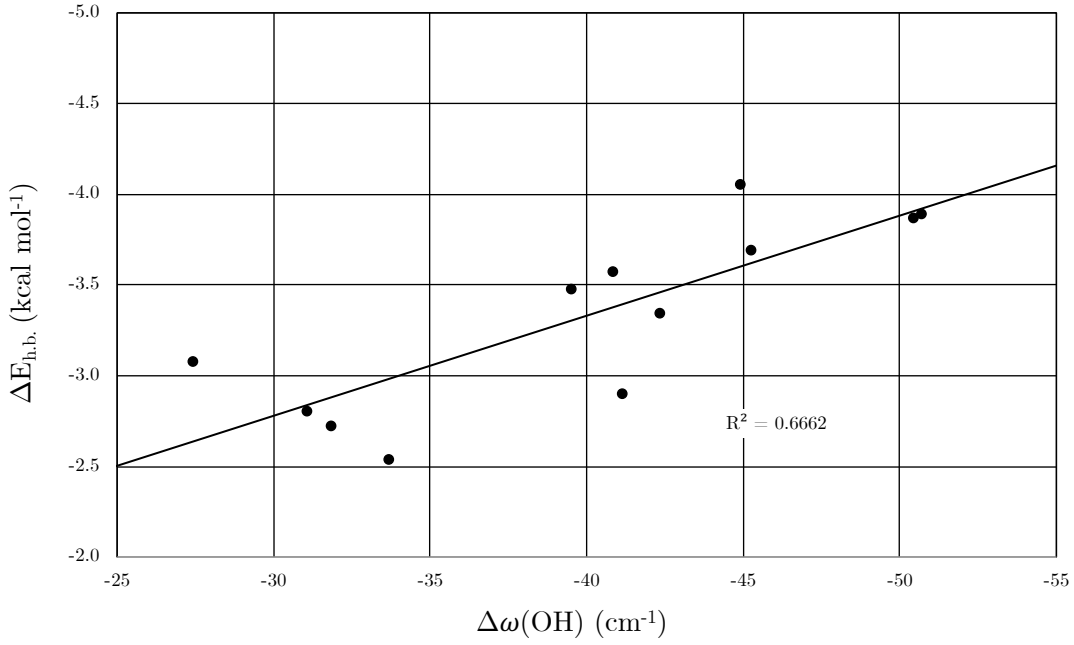

Figure S11: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($\Delta E_{h.b.}$ in kcal mol^{-1} as defined by Equation 3) versus the corresponding changes in the harmonic OH stretching frequencies ($\Delta\omega$(OH) in cm^{-1}). Trend lines and coefficients of determination are shown when $r^2 > 0.5$.

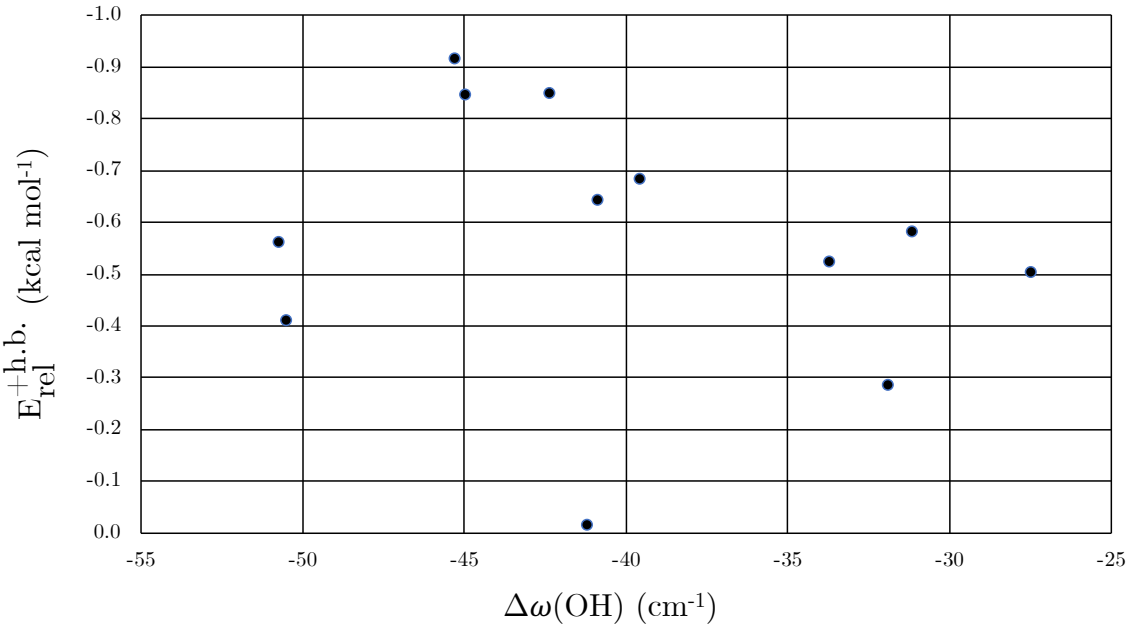

Figure S12: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($E_{rel}^{+h.b.}$ in kcal mol^{-1} as defined by Equation 2) versus the corresponding changes in the harmonic OH stretching frequencies ($\Delta\omega$(OH) in cm^{-1}). Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

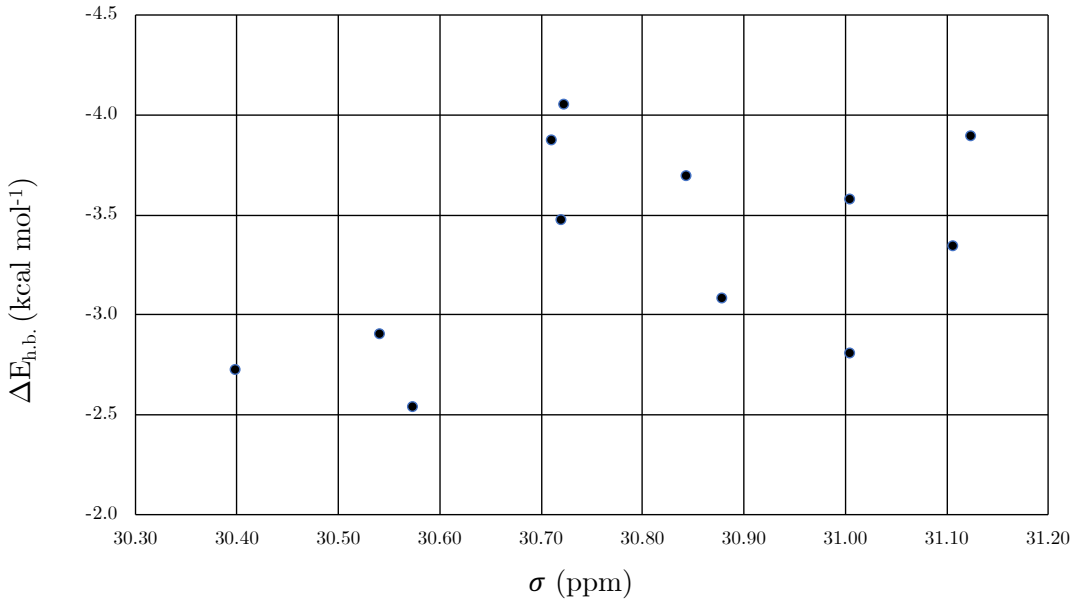

Figure S13: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($\Delta E_{h.b.}$ in kcal mol^{-1} as defined by Equation 3) versus the *cis*+h.b. isotropic NMR chemical shielding constants for the hydroxyl H atom (σ in ppm). Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

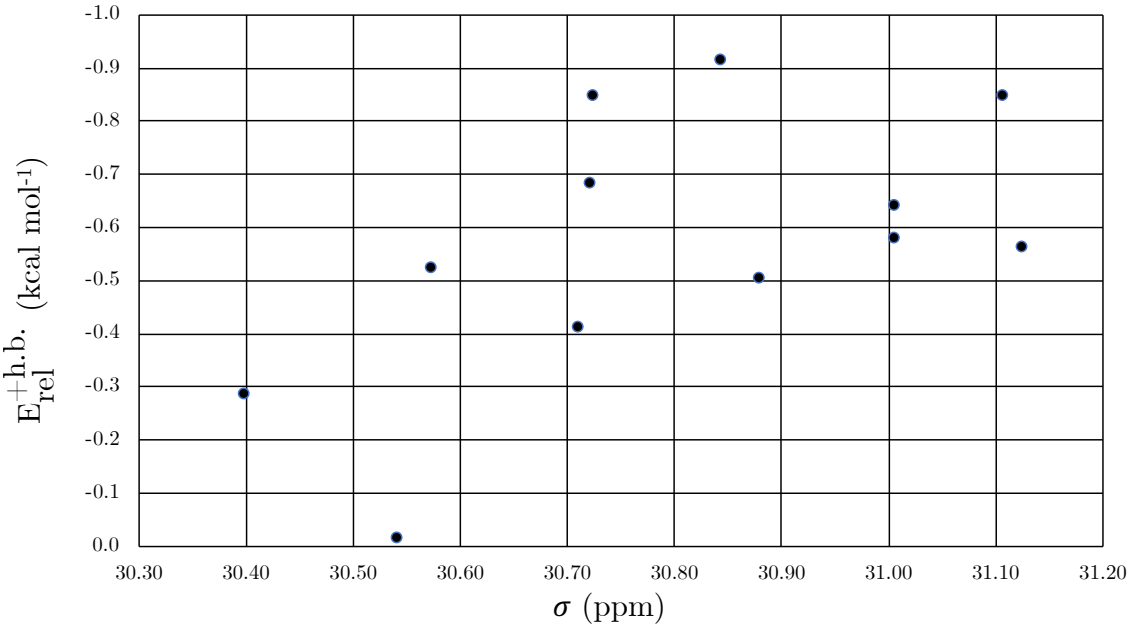

Figure S14: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($E_{rel}^{+h.b.}$ in kcal mol^{-1} as defined by Equation 2) versus the *cis*+h.b. isotropic NMR chemical shielding constants for the hydroxyl H atom (σ in ppm). Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

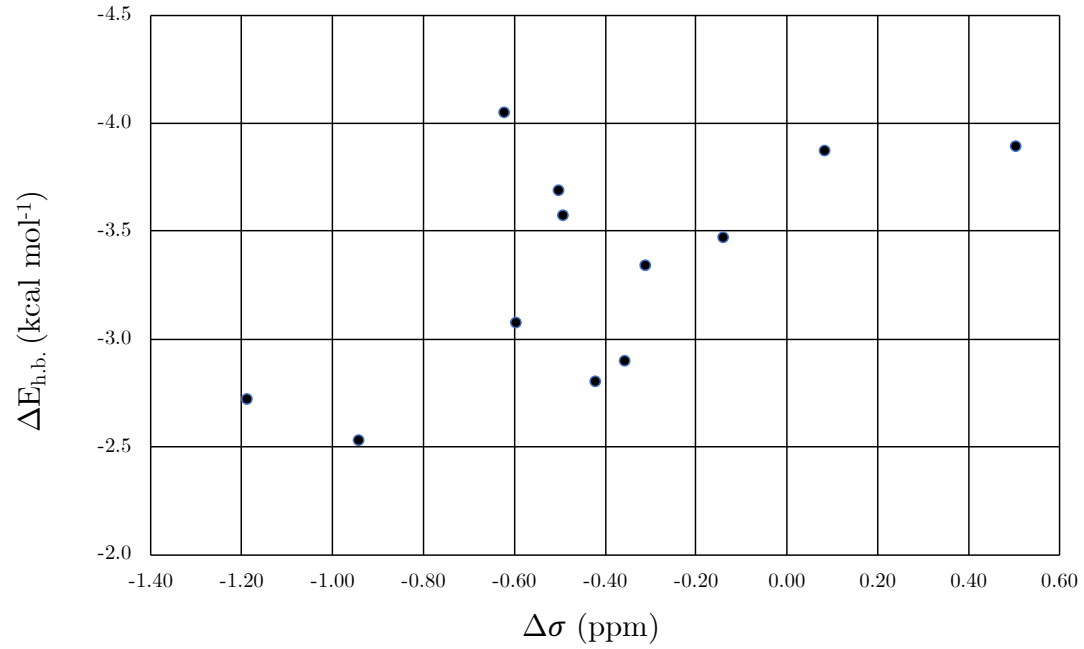

Figure S15: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($\Delta E_{h.b.}$ in kcal mol^{-1} as defined by Equation 3) versus the corresponding changes in the isotropic NMR chemical shielding constants for the hydroxyl H atom ($\Delta\sigma$ in ppm). Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

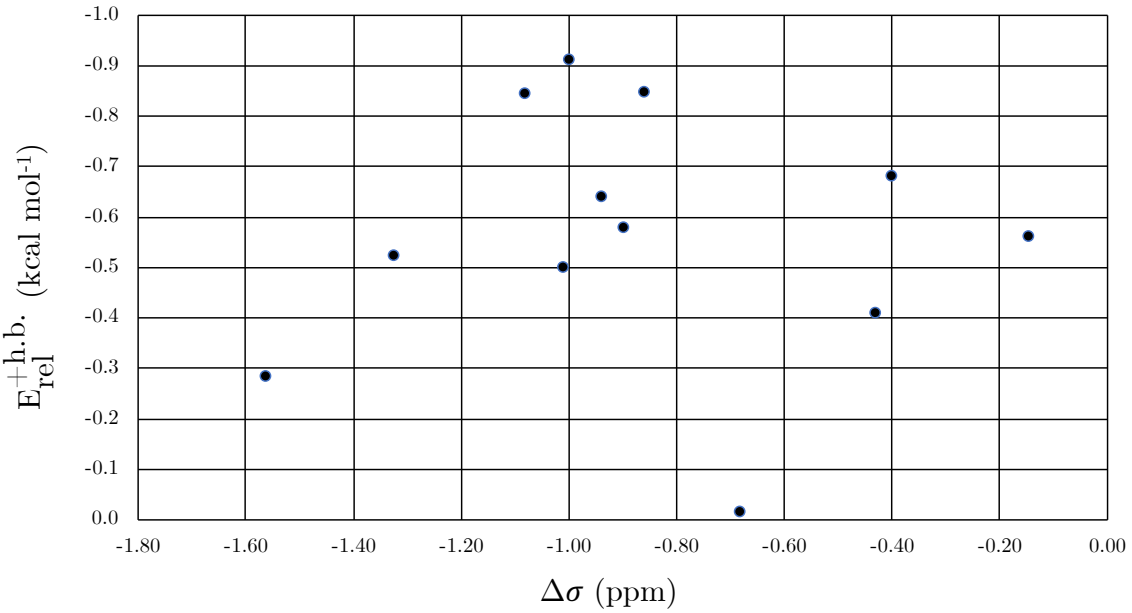

Figure S16: M06-2X/TZ relative electronic energies of the *cis*+h.b. structures ($E_{rel}^{+h.b.}$ in kcal mol^{-1} as defined by Equation 2) versus the corresponding changes in the isotropic NMR chemical shielding constants for the hydroxyl H atom ($\Delta\sigma$ in ppm). Trend lines and coefficients of determination are not shown when $r^2 < 0.5$.

Table S10: M06-2X optimized geometry of *cis*-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.257707	0.783401	0.023501
C	1.555838	0.187343	0.350531
C	1.430101	−1.316467	0.425951
C	0.123092	−1.588119	−0.335669
C	−0.756641	−0.345461	−0.099039
C	−1.566261	−0.468483	1.186701
H	−2.239359	−1.325524	1.120141
H	−0.914940	−0.618912	2.049321
H	−2.165522	0.425936	1.349861
O	−1.610321	−0.053383	−1.192309
H	−2.263680	−0.753724	−1.270069
H	0.323072	−1.650529	−1.402719
H	−0.371117	−2.505660	−0.016729
H	2.285192	−1.828065	−0.014829
H	1.359642	−1.622387	1.471721
O	1.288007	0.688413	−0.953779
H	2.313497	0.723515	0.908871
C	−0.186496	2.168070	0.379261
H	−0.614616	2.202539	1.380491
H	0.663493	2.846082	0.337191
H	−0.941187	2.504788	−0.331969

Table S11: M06-2X optimized geometry of *cis*-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.018659	−0.003960	0.020192
C	1.526907	−0.031572	0.022235
C	1.982671	1.434395	0.015061
C	0.855625	2.141364	−0.698264
C	−0.351005	1.317219	−0.666379
C	−1.758863	1.820755	−0.717933
H	−2.415337	1.045402	−1.115205
H	−2.113695	2.093131	0.275473
H	−1.814680	2.694687	−1.363873
O	0.414365	1.451721	−1.868034
H	0.814239	3.221685	−0.762574
H	2.066016	1.835291	1.027268
H	2.944169	1.573789	−0.478192
H	1.915835	−0.596758	0.867110
H	1.861265	−0.523472	−0.889503
O	−0.578319	−1.098214	−0.684220
H	−0.269862	−1.040915	−1.594991
C	−0.592203	−0.053746	1.423381
H	−0.304556	−0.990604	1.898396
H	−0.213784	0.775826	2.022698
H	−1.679648	−0.002979	1.394568

Table S12: M06-2X optimized geometry of *trans*-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	0.724709	−0.411326	0.005455
C	−0.228458	−1.587610	0.280719
C	−1.570646	−1.183894	−0.348661
C	−1.566362	0.318299	−0.217065
C	−0.199550	0.800157	−0.015101
O	−1.124149	0.764707	1.066146
H	−2.328335	0.932729	−0.679865
H	−1.604658	−1.442717	−1.407632
H	−2.422662	−1.648393	0.146468
H	0.175099	−2.511972	−0.132194
H	−0.343889	−1.717250	1.354971
C	0.324530	2.141380	−0.418269
H	−0.491807	2.858745	−0.477817
H	1.044317	2.503844	0.317371
H	0.820879	2.072957	−1.384305
C	1.845109	−0.293867	1.021539
H	2.415062	−1.224395	1.073482
H	2.525265	0.511382	0.744558
H	1.435716	−0.089996	2.010890
O	1.240252	−0.481898	−1.322745
H	1.870299	−1.206222	−1.364824

Table S13: M06-2X optimized geometry of *cis*-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.919335	0.587805	−0.105864
C	−1.714982	−0.547726	−0.580181
C	−0.910517	−1.821030	−0.469953
C	0.193213	−1.441145	0.529669
C	0.450601	0.063094	0.309093
C	1.466448	0.323903	−0.809881
C	2.890346	−0.094544	−0.462711
H	2.966012	−1.158480	−0.238236
H	3.563572	0.111686	−1.293433
H	3.260766	0.465060	0.396840
H	1.131757	−0.191968	−1.714265
H	1.461957	1.392150	−1.030104
O	0.834487	0.740452	1.494536
H	1.585419	0.285089	1.883443
H	−0.175048	−1.564986	1.545648
H	1.091854	−2.043897	0.411116
H	−1.509907	−2.664286	−0.127897
H	−0.498936	−2.077733	−1.448093
O	−1.965520	0.040491	0.690186
H	−2.506030	−0.434995	−1.311508
C	−1.100621	2.014742	−0.524215
H	−0.586807	2.227141	−1.460654
H	−2.161428	2.219954	−0.653055
H	−0.705771	2.677121	0.246750

Table S14: M06-2X optimized geometry of *cis*-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.426520	0.099420	0.662900
C	−0.652340	0.602520	−0.291320
C	−1.373630	−0.542420	−0.844730
C	−0.757220	−1.831560	−0.362850
C	0.080290	−1.399430	0.852190
H	0.977360	−2.003150	0.983310
H	−0.510290	−1.493920	1.761350
H	−0.137140	−2.246080	−1.158950
H	−1.511070	−2.575550	−0.105970
O	−1.940670	0.230810	0.212300
H	−1.905950	−0.487310	−1.786630
C	−0.555070	1.961750	−0.908560
H	−1.475390	2.193480	−1.441010
H	−0.400250	2.709880	−0.129820
H	0.280730	2.017430	−1.605990
O	0.366310	0.816900	1.884570
H	−0.543150	0.766280	2.198910
C	1.830770	0.330480	0.121310
C	2.120020	−0.382360	−1.194060
H	1.400950	−0.108560	−1.968380
H	3.113420	−0.125820	−1.558520
H	2.084390	−1.465730	−1.076350
H	1.975240	1.406940	0.012300
H	2.529970	0.000050	0.891510

Table S15: M06-2X optimized geometry of *trans*-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	−0.466810	−0.011006	0.210317
C	0.887405	0.635761	−0.057835
C	1.903359	−0.416542	−0.034021
C	1.260645	−1.747127	0.261963
C	−0.217233	−1.502761	−0.081207
H	−0.892634	−2.133212	0.496717
H	−0.392966	−1.700320	−1.137421
H	1.388237	−1.969842	1.322050
H	1.694004	−2.563532	−0.314768
O	1.462958	0.154154	−1.267478
H	2.934718	−0.212055	0.224679
C	1.115784	2.075621	0.276337
H	2.164752	2.329382	0.135133
H	0.519372	2.716286	−0.374882
H	0.830187	2.268414	1.308690
C	−1.583112	0.601170	−0.626394
C	−2.929122	−0.091624	−0.445971
H	−2.878304	−1.141821	−0.734652
H	−3.271270	−0.040242	0.589835
H	−3.696283	0.383167	−1.055630
H	−1.672484	1.654783	−0.353893
H	−1.277645	0.558670	−1.674106
O	−0.684835	0.199731	1.604233
H	−1.500330	−0.241547	1.855064

Table S16: M06-2X optimized geometry of *cis*-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.397314	−0.292295	0.373495
C	0.080917	−1.566391	−0.173497
C	1.418305	−1.370674	−0.849021
C	1.915653	−0.049653	−0.241718
C	0.646346	0.772170	0.058084
C	0.223650	1.607817	−1.143875
H	1.005668	2.332839	−1.379130
H	0.066946	0.984512	−2.025688
H	−0.694414	2.153378	−0.928589
O	0.780442	1.600020	1.201488
H	1.415993	2.294097	1.007073
H	2.412799	−0.242664	0.705881
H	2.603276	0.485625	−0.896322
H	2.102446	−2.198723	−0.665737
H	1.271117	−1.290289	−1.927954
O	0.135437	−1.306468	1.222428
H	−0.594946	−2.358036	−0.473396
C	−1.841911	0.079003	0.594352
C	−2.711145	0.000168	−0.658982
H	−2.714896	−1.012186	−1.063507
H	−3.741106	0.271100	−0.429125
H	−2.359086	0.668684	−1.443120
H	−2.231906	−0.600233	1.352025
H	−1.875678	1.082817	1.023193

Table S17: M06-2X optimized geometry of *cis*-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−1.845264	−0.014939	0.595361
C	−0.390291	−0.311371	0.348504
C	0.137800	−1.572330	−0.171262
C	1.431841	−1.325640	−0.908389
C	1.895804	0.028599	−0.354342
C	0.615089	0.798161	0.047337
C	0.138400	1.722117	−1.056327
H	−0.787127	2.219523	−0.768642
H	0.895837	2.484911	−1.232214
H	−0.025929	1.168573	−1.981850
O	0.812587	1.613761	1.189169
H	1.046131	1.030333	1.919450
H	2.495192	−0.126874	0.540711
H	2.496805	0.596182	−1.062339
H	2.163102	−2.117722	−0.749821
H	1.223097	−1.273371	−1.978898
O	0.221084	−1.271861	1.220738
H	−0.504716	−2.408504	−0.419264
H	−2.208070	−0.759030	1.304772
H	−1.920483	0.957570	1.087789
C	−2.707654	−0.046291	−0.664658
H	−2.388361	0.694174	−1.395854
H	−2.659170	−1.026342	−1.140011
H	−3.749886	0.155677	−0.420514

Table S18: M06-2X optimized geometry of *trans*-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	0.557678	0.797773	−0.018912
C	1.889144	0.081243	−0.312846
C	1.505105	−1.321498	−0.806793
C	0.220107	−1.595969	−0.066691
C	−0.378980	−0.337859	0.383169
C	−1.854256	−0.129501	0.593710
H	−2.007212	0.767604	1.198773
C	−2.665042	−0.036645	−0.696588
H	−2.509549	−0.924932	−1.309987
H	−3.728676	0.034491	−0.471072
H	−2.372533	0.829445	−1.283449
H	−2.201312	−0.972227	1.193385
O	0.275409	−1.207928	1.305518
H	−0.379666	−2.474223	−0.272295
H	1.300878	−1.322792	−1.878276
H	2.276588	−2.063115	−0.602649
H	2.470871	0.644689	−1.042255
H	2.472166	0.007140	0.602783
C	0.683359	1.870592	1.046981
H	0.969558	1.423474	1.998672
H	1.449248	2.597773	0.767248
H	−0.261997	2.398333	1.170293
O	0.003741	1.333798	−1.219152
H	0.545624	2.078588	−1.494048

Table S19: M06-2X optimized geometry of *cis*-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.970972	0.007922	0.224872
C	−0.330233	0.607568	−0.292114
C	−1.106667	−0.479796	−0.922787
C	−0.344802	−1.782364	−0.806068
C	0.655747	−1.497394	0.325768
C	−0.361893	2.041166	−0.733923
N	−1.493866	0.040110	0.395380
C	2.108116	0.268013	−0.757671
O	1.268300	0.598801	1.479778
H	3.011133	−0.246699	−0.423492
H	1.859206	−0.101905	−1.753839
H	2.326163	1.332950	−0.821821
H	2.088898	0.222902	1.809489
H	0.182209	−1.668960	1.289216
H	1.556210	−2.108419	0.259471
H	−0.994368	−2.627692	−0.579929
H	0.168094	−1.993260	−1.746490
H	−1.750131	−0.286485	−1.770958
H	0.322840	2.221948	−1.561993
H	−1.364511	2.315934	−1.063599
H	−0.078573	2.693020	0.093687
H	−2.274758	0.679418	0.296589

Table S20: M06-2X optimized geometry of *cis*-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.301646	−0.754350	−0.055112
C	−0.788641	0.302371	0.118797
C	0.000449	1.628529	0.234225
C	1.320376	1.414362	−0.519702
C	1.564369	−0.070957	−0.381727
C	−0.061511	−2.141016	−0.494167
C	−1.747358	0.316732	−1.056376
N	1.321342	−0.562632	0.987325
O	−1.565317	0.039107	1.273594
H	−0.798598	−2.569788	0.187093
H	−0.486780	−2.140691	−1.497411
H	0.818981	−2.784675	−0.502355
H	2.327438	−0.562840	−0.970491
H	1.217838	1.661360	−1.578232
H	2.133811	2.014894	−0.112966
H	−0.576015	2.470711	−0.144752
H	0.205211	1.810250	1.287364
H	−0.941766	−0.054298	2.003104
H	−2.476104	1.114407	−0.919356
H	−1.207422	0.489704	−1.988861
H	−2.283666	−0.628494	−1.127133
H	1.824145	−1.432629	1.125097

Table S21: M06-2X optimized geometry of *trans*-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
N	−1.175409	0.692722	1.102511
C	−1.568682	0.254708	−0.248791
C	−1.479835	−1.243694	−0.417532
C	−0.132047	−1.587410	0.236145
C	0.760781	−0.356286	0.002138
C	−0.222449	0.807332	−0.005288
C	1.864476	−0.208535	1.032407
O	1.297904	−0.377393	−1.321326
C	0.240448	2.155415	−0.469330
H	−2.314897	0.829832	−0.780297
H	−1.467648	−1.481144	−1.481773
H	−2.311987	−1.772627	0.046225
H	0.329951	−2.481831	−0.182690
H	−0.264288	−1.739357	1.305178
H	−0.605180	2.838404	−0.560320
H	0.949804	2.587438	0.239612
H	0.730645	2.073805	−1.437408
H	2.486666	−1.106110	1.061513
H	2.501113	0.641543	0.786486
H	1.432681	−0.058936	2.021648
H	1.933656	−1.095705	−1.375543
H	−1.570189	1.608221	1.289174

Table S22: M06-2X optimized geometry of *cis*-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
N	−1.997241	−0.000316	0.685301
C	−0.919628	0.601231	−0.106554
C	0.443700	0.045340	0.294841
C	0.176421	−1.467184	0.430760
C	−0.906566	−1.787895	−0.611651
C	−1.716960	−0.511596	−0.662450
C	−1.048508	2.031917	−0.543372
C	1.478258	0.356467	−0.794704
C	2.884770	−0.137794	−0.478135
O	0.830431	0.653174	1.518012
H	2.931090	−1.221761	−0.376962
H	3.577316	0.144944	−1.269783
H	3.253023	0.309192	0.446015
H	1.132108	−0.069077	−1.740981
H	1.514589	1.438782	−0.923926
H	1.526720	0.127436	1.919022
H	−0.217668	−1.640182	1.429592
H	1.075149	−2.067614	0.301037
H	−1.505281	−2.653797	−0.329623
H	−0.468395	−1.985421	−1.591903
H	−2.440656	−0.342596	−1.448941
H	−0.480091	2.232760	−1.450526
H	−2.092919	2.271905	−0.746285
H	−0.688025	2.697207	0.242621
H	−2.803223	0.614322	0.659344

Table S23: M06-2X optimized geometry of *cis*-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
N	−1.961265	0.074979	0.724283
C	−0.926095	0.610798	−0.174227
C	0.433095	0.051550	0.252674
C	0.177977	−1.472303	0.363263
C	−0.981809	−1.791090	−0.590357
C	−1.775805	−0.506459	−0.617790
C	−1.042592	2.019761	−0.674651
C	1.516533	0.404101	−0.761017
C	2.903376	−0.101988	−0.383134
O	0.832342	0.616978	1.489722
H	2.957633	−1.189918	−0.386010
H	3.648329	0.264973	−1.088190
H	3.170866	0.247207	0.612387
H	1.215424	0.014015	−1.737910
H	1.551776	1.491461	−0.846760
H	0.096759	0.481271	2.097919
H	−0.120184	−1.688724	1.387045
H	1.070085	−2.056165	0.150692
H	−1.570852	−2.644973	−0.256021
H	−0.619477	−2.006966	−1.597452
H	−2.557104	−0.354295	−1.350813
H	−0.509449	2.154854	−1.615076
H	−2.088602	2.279584	−0.842293
H	−0.625604	2.714776	0.056386
H	−2.764217	0.694461	0.713151

Table S24: M06-2X optimized geometry of *trans*-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
N	1.483849	0.103015	−1.302289
C	0.894161	0.640998	−0.072608
C	−0.461172	0.002293	0.206294
C	−0.212027	−1.499262	−0.029877
C	1.259520	−1.733638	0.348210
C	1.917244	−0.418646	0.005945
C	−1.574434	0.585011	−0.655071
C	−2.925407	−0.089627	−0.445889
O	−0.694438	0.254438	1.592792
C	1.125377	2.071170	0.313565
H	−0.899337	−2.108886	0.557085
H	−0.368149	−1.729783	−1.082157
H	1.361384	−1.913867	1.418917
H	1.693638	−2.577602	−0.187222
H	2.920197	−0.195143	0.344059
H	2.179962	2.328510	0.206100
H	0.546404	2.744803	−0.321326
H	0.828624	2.235430	1.347632
H	−2.880417	−1.152269	−0.686462
H	−3.268203	0.011465	0.586003
H	−3.688951	0.361037	−1.078280
H	−1.657693	1.650063	−0.427223
H	−1.266567	0.494499	−1.698625
H	−1.491474	−0.212869	1.854899
H	2.172918	0.761408	−1.649501

Table S25: M06-2X optimized geometry of *cis*-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
N	−0.233528	−1.411638	−1.158806
C	0.387396	−0.338805	−0.370799
C	−0.628793	0.755045	−0.059803
C	−1.888186	−0.030133	0.357526
C	−1.368534	−1.312649	1.027065
C	−0.073877	−1.579368	0.289704
C	1.837535	0.024947	−0.601223
C	2.715408	−0.007068	0.648528
C	−0.147181	1.655997	1.071805
O	−0.818246	1.525448	−1.236321
H	−0.914371	2.399931	1.297013
H	0.041701	1.083592	1.981224
H	0.763782	2.181824	0.787948
H	−1.445964	2.227535	−1.045409
H	−2.433304	−0.281597	−0.548717
H	−2.535927	0.555794	1.010026
H	−2.075189	−2.137995	0.941987
H	−1.161783	−1.153026	2.087206
H	0.630425	−2.314483	0.656255
H	2.724587	−1.004258	1.089143
H	3.743565	0.258890	0.403280
H	2.364468	0.686633	1.410083
H	2.256920	−0.662262	−1.338949
H	1.867104	1.014160	−1.063657
H	0.496273	−1.921892	−1.643287

Table S26: M06-2X optimized geometry of *cis*-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
N	0.253964	−1.319030	1.236671
C	−0.406237	−0.338863	0.355266
C	0.610243	0.761327	0.036671
C	1.862603	−0.019425	−0.433115
C	1.359135	−1.359022	−0.988019
C	0.094691	−1.609217	−0.198630
C	−1.865658	−0.011293	0.556742
C	−2.697651	−0.005402	−0.724278
C	0.124297	1.726753	−1.027001
O	0.868837	1.541026	1.190782
H	−0.783072	2.236143	−0.704191
H	0.894054	2.478090	−1.198936
H	−0.071779	1.204081	−1.964106
H	1.094863	0.917167	1.890668
H	2.496127	−0.196019	0.433522
H	2.439584	0.551888	−1.158388
H	2.092394	−2.157384	−0.874969
H	1.107287	−1.281518	−2.047661
H	−0.586405	−2.400470	−0.484070
H	−2.294012	−0.744018	1.244967
H	−1.932860	0.955966	1.061213
H	−2.350861	0.745308	−1.430942
H	−2.648086	−0.975949	−1.218790
H	−3.743552	0.204437	−0.501638
H	−0.452865	−1.824575	1.758983

Table S27: M06-2X optimized geometry of *trans*-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
N	0.241360	−1.180391	1.375337
C	0.057740	−1.600563	−0.023111
C	1.317295	−1.444776	−0.842158
C	1.845908	−0.070776	−0.402758
C	0.596624	0.764178	−0.062256
C	−0.412555	−0.273551	0.421666
C	0.870906	1.853265	0.958360
O	0.035469	1.319321	−1.252731
C	−1.871257	0.075309	0.591605
C	−2.671763	0.131651	−0.707712
H	−1.952094	1.028475	1.120501
H	−2.588556	−0.812354	−1.247506
H	−3.726664	0.307414	−0.496647
H	−2.306560	0.921513	−1.356967
H	−2.317213	−0.675793	1.249500
H	−0.647319	−2.393864	−0.234478
H	1.055035	−1.441489	−1.900828
H	2.039553	−2.241541	−0.666385
H	2.436657	0.424912	−1.173591
H	2.463405	−0.176879	0.486270
H	1.181105	1.408158	1.903060
H	1.669885	2.511947	0.609604
H	−0.021961	2.457008	1.121058
H	0.646427	1.980586	−1.589040
H	−0.468555	−1.614756	1.954320

Table S28: M06-2X optimized geometry of *cis*-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.980181	−0.011698	0.249408
C	−0.343303	0.591596	−0.230557
C	−1.116803	−0.507470	−0.883629
C	−0.292046	−1.784831	−0.835451
C	0.701997	−1.526049	0.302287
C	−0.320284	1.995780	−0.775894
P	−1.814127	0.013846	0.772373
C	2.104633	0.294480	−0.737480
O	1.298743	0.534681	1.519816
H	3.015084	−0.224200	−0.429463
H	1.850339	−0.042230	−1.743611
H	2.310614	1.362864	−0.766938
H	2.182524	0.247266	1.764937
H	0.247417	−1.752642	1.267343
H	1.614865	−2.115033	0.214319
H	−0.894372	−2.677244	−0.670951
H	0.235426	−1.911326	−1.784110
H	−1.710323	−0.297344	−1.762935
H	0.303031	2.059231	−1.670571
H	−1.322293	2.325062	−1.045191
H	0.077462	2.685736	−0.030965
H	−2.690681	0.976302	0.216826

Table S29: M06-2X optimized geometry of *cis*-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.969753	−0.000071	0.241285
C	−0.341864	0.599669	−0.294699
C	−1.106794	−0.501494	−0.938017
C	−0.288177	−1.781752	−0.857913
C	0.687521	−1.515642	0.292767
C	−0.306928	1.997521	−0.853517
P	−1.839123	0.036900	0.699380
C	2.128966	0.300259	−0.698147
O	1.350036	0.535595	1.494112
H	3.023632	−0.198334	−0.327618
H	1.916474	−0.057064	−1.706506
H	2.324483	1.370111	−0.734866
H	0.587864	0.481021	2.080714
H	0.218575	−1.752984	1.249623
H	1.604387	−2.098251	0.226220
H	−0.898085	−2.669673	−0.698304
H	0.254429	−1.916047	−1.796640
H	−1.697474	−0.305238	−1.822644
H	0.333088	2.043837	−1.737015
H	−1.302083	2.330212	−1.143572
H	0.085998	2.694635	−0.112539
H	−2.700657	1.007965	0.140067

Table S30: M06-2X optimized geometry of *trans*-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	−0.301998	0.610113	−0.272068
C	1.028557	−0.009432	0.168549
C	0.700947	−1.498400	0.357114
C	−0.346401	−1.796336	−0.722373
C	−1.137559	−0.502491	−0.813277
C	1.657900	0.642476	1.385620
O	1.884776	0.143408	−0.968390
P	−1.743863	0.152930	0.831970
C	−0.250625	1.967135	−0.923832
H	−1.768024	−0.328637	−1.674290
H	0.147089	−1.972856	−1.679444
H	−0.961269	−2.663478	−0.486547
H	1.598942	−2.109725	0.266732
H	0.286391	−1.665524	1.352832
H	−1.232426	2.245985	−1.304352
H	0.063803	2.734929	−0.215679
H	0.457487	1.954358	−1.751916
H	2.595363	0.143297	1.642060
H	1.874828	1.690794	1.181313
H	0.991969	0.580109	2.245498
H	2.746265	−0.219161	−0.744240
H	−2.607859	1.117057	0.261481

Table S31: M06-2X optimized geometry of *cis*-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.406318	−1.476309	0.330985
C	0.639096	0.047509	0.290452
C	−0.680081	0.599536	−0.267754
C	−1.376417	−0.527092	−0.959401
C	−0.508844	−1.771353	−0.862315
C	1.803206	0.422049	−0.640429
C	3.170074	−0.069325	−0.175417
O	0.853350	0.604250	1.578394
C	−0.695801	2.003429	−0.817095
P	−2.180571	−0.034783	0.655986
H	3.220338	−1.154722	−0.096360
H	3.942305	0.241214	−0.877965
H	3.436698	0.357389	0.792833
H	1.589664	0.037661	−1.641618
H	1.835783	1.508736	−0.715853
H	1.649743	0.218263	1.952199
H	−0.101720	−1.712091	1.266937
H	1.331383	−2.049039	0.305621
H	−1.084291	−2.686799	−0.730880
H	0.077809	−1.877277	−1.778249
H	−1.927217	−0.338753	−1.870921
H	−0.052887	2.091819	−1.695183
H	−1.702734	2.289805	−1.115235
H	−0.349078	2.711660	−0.063801
H	−3.063356	0.893630	0.054674

Table S32: M06-2X optimized geometry of *cis*-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.365506	1.473232	0.738952
C	−0.569109	−0.057974	0.673385
C	0.480742	−0.526909	−0.349725
C	0.961245	0.661516	−1.102266
C	0.215513	1.896154	−0.617866
O	−0.405684	−0.681667	1.935475
C	−1.991386	−0.438985	0.256555
C	−2.488316	0.186221	−1.040490
C	0.306552	−1.882152	−0.983771
P	2.219190	0.030009	0.129018
H	−1.290483	1.991660	0.988786
H	0.346936	1.686496	1.537494
H	−0.577233	2.133772	−1.327682
H	0.859905	2.770716	−0.538169
H	1.215232	0.574621	−2.150362
H	1.136906	−2.113125	−1.649034
H	0.256142	−2.656378	−0.217347
H	−0.614494	−1.925783	−1.568733
H	0.524669	−0.618732	2.177086
H	−1.803628	0.004910	−1.870974
H	−3.457739	−0.228887	−1.312641
H	−2.612323	1.264452	−0.941335
H	−2.041303	−1.527022	0.201010
H	−2.641397	−0.144721	1.082553
H	2.859935	−0.854423	−0.768287

Table S33: M06-2X optimized geometry of *trans*-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
P	1.645722	0.077625	−1.764594
C	0.886648	0.630195	−0.143863
C	−0.473132	−0.013960	0.150446
C	−0.223074	−1.517825	−0.052992
C	1.224531	−1.729506	0.407830
C	1.917667	−0.437432	0.013601
C	−1.615878	0.552796	−0.684750
C	−2.971376	−0.070735	−0.371425
O	−0.691498	0.242910	1.541335
C	1.109133	2.034941	0.353394
H	−0.937376	−2.120884	0.507289
H	−0.334274	−1.773734	−1.108706
H	1.256628	−1.826419	1.494301
H	1.679932	−2.616650	−0.029609
H	2.874634	−0.196084	0.455311
H	2.147308	2.330901	0.207497
H	0.480124	2.749812	−0.178349
H	0.872428	2.093823	1.415459
H	−2.963215	−1.148434	−0.539700
H	−3.269019	0.112598	0.662650
H	−3.748979	0.355119	−1.003715
H	−1.658836	1.630209	−0.512098
H	−1.374355	0.403802	−1.738651
H	−1.480115	−0.233217	1.814408
H	2.641383	1.082697	−1.750097

Table S34: M06-2X optimized geometry of *cis*-2-ethyl-2,3-phosphirane–methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.317919	1.018819	−0.311864
C	0.328843	−0.368214	−0.198181
C	−0.290587	−1.044766	0.984005
C	−1.278061	−0.088154	1.634858
C	−1.616233	0.895540	0.509225
C	1.798087	−0.508800	−0.562803
C	2.767403	−0.304103	0.601905
P	−0.873667	−1.735628	−0.650258
C	0.570077	2.114710	0.273270
O	−0.554598	1.291056	−1.684974
H	1.518368	2.177868	−0.257945
H	0.060463	3.076754	0.180711
H	0.766360	1.943823	1.331872
H	−0.843939	2.203413	−1.771924
H	−2.391090	0.484695	−0.138724
H	−1.962492	1.861753	0.876035
H	−2.159736	−0.589747	2.031686
H	−0.788892	0.429581	2.463849
H	0.304766	−1.690175	1.614560
H	1.979766	−1.496541	−0.983556
H	2.008666	0.199453	−1.367210
H	2.677091	0.683388	1.049577
H	2.590174	−1.040806	1.385906
H	3.796776	−0.423967	0.263728
H	0.131479	−2.730866	−0.703635

Table S35: M06-2X optimized geometry of *cis*-2-ethyl-2,3-phosphirane-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.365889	0.999877	−0.267727
C	0.302390	−0.384251	−0.142655
C	−0.291710	−1.058748	1.043967
C	−1.271282	−0.105055	1.712171
C	−1.639666	0.874762	0.594049
C	1.762516	−0.524025	−0.538028
C	2.750165	−0.280097	0.603423
P	−0.912564	−1.765504	−0.572097
C	0.519566	2.117772	0.264711
O	−0.635248	1.352553	−1.611431
H	1.456847	2.170681	−0.286333
H	−0.006083	3.062972	0.133751
H	0.733391	1.978063	1.324187
H	−1.078791	0.605690	−2.028028
H	−2.443242	0.464852	−0.020390
H	−1.972384	1.844015	0.960814
H	−2.138650	−0.611124	2.133521
H	−0.761326	0.415639	2.526376
H	0.310405	−1.712100	1.660225
H	1.945303	−1.520665	−0.937362
H	1.950354	0.168664	−1.361655
H	2.652378	0.716425	1.028216
H	2.597542	−1.001147	1.406924
H	3.774373	−0.393635	0.248269
H	0.091634	−2.755101	−0.668920

Table S36: M06-2X optimized geometry of *trans*-2-ethyl-2,3-phosphirane-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	−0.368458	−0.295732	0.248356
C	0.460238	0.996151	0.192808
C	1.684435	0.623009	−0.658807
C	1.154904	−0.400944	−1.667820
C	0.100966	−1.158377	−0.878948
C	0.820245	1.575399	1.549339
O	−0.354484	1.927221	−0.527607
P	0.657987	−1.766781	0.797895
C	−1.835557	−0.176321	0.629458
C	−2.763628	0.085322	−0.556123
H	−1.934248	0.633828	1.354640
H	−2.733615	−0.744219	−1.263300
H	−3.793780	0.189088	−0.214383
H	−2.475793	0.992473	−1.080481
H	−2.159351	−1.083536	1.139140
H	−0.606705	−1.777987	−1.411388
H	0.667539	0.112184	−2.498984
H	1.938206	−1.041796	−2.069745
H	2.115040	1.508039	−1.127060
H	2.454000	0.175078	−0.027680
H	1.413024	0.868574	2.128144
H	1.404547	2.490580	1.425640
H	−0.081757	1.820999	2.109530
H	0.102998	2.772624	−0.544706
H	−0.463590	−2.606887	0.989258

Table S37: M06-2X optimized geometry of *cis*-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.266651	0.791570	0.050147
C	−1.575606	0.194592	−0.305768
C	−1.415763	−1.308267	−0.448306
C	−0.117836	−1.613698	0.310273
C	0.748377	−0.350682	0.142920
C	1.569606	−0.425478	−1.143419
H	2.227156	−1.296260	−1.106797
H	0.926747	−0.528207	−2.019371
H	2.184357	0.465017	−1.260182
O	1.602730	−0.105898	1.245161
H	2.292671	−0.774774	1.254917
H	−0.318388	−1.748880	1.370295
H	0.386528	−2.503980	−0.064845
H	−2.270976	−1.861809	−0.064684
H	−1.312917	−1.548573	−1.509740
S	−1.490458	0.817439	1.398326
H	−2.254880	0.727425	−0.958124
C	0.191361	2.127853	−0.468473
H	0.523551	2.050294	−1.505067
H	−0.620963	2.849310	−0.417444
H	1.021822	2.496374	0.133770

Table S38: M06-2X optimized geometry of *cis*-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.010287	−0.026340	−0.018720
C	1.532685	−0.040610	0.038545
C	1.957812	1.431143	0.046487
C	0.859316	2.136071	−0.725404
C	−0.349932	1.290459	−0.739067
C	−1.744307	1.843250	−0.638131
H	−2.467788	1.095053	−0.962692
H	−1.974219	2.117636	0.392624
H	−1.849852	2.725215	−1.266011
S	0.475912	1.438318	−2.367923
H	0.769221	3.213103	−0.672661
H	1.966433	1.828883	1.064657
H	2.945919	1.592950	−0.380405
H	1.891903	−0.590004	0.906590
H	1.912998	−0.537863	−0.851663
O	−0.549194	−1.153291	−0.675599
H	−0.228172	−1.135009	−1.584420
C	−0.608301	−0.033037	1.380434
H	−0.301686	−0.944422	1.891336
H	−0.262555	0.827046	1.955943
H	−1.695428	−0.015509	1.333293

Table S39: M06-2X optimized geometry of *trans*-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	0.721591	−0.397856	0.058979
C	−0.219542	−1.593338	0.276318
C	−1.539890	−1.174462	−0.382154
C	−1.577453	0.328294	−0.193776
C	−0.206499	0.823021	0.064587
S	−1.310244	0.918067	1.510372
H	−2.266785	0.927763	−0.772952
H	−1.510706	−1.377922	−1.454410
H	−2.406468	−1.679873	0.039787
H	0.203613	−2.496254	−0.163980
H	−0.360043	−1.769459	1.340540
C	0.314312	2.117142	−0.496524
H	−0.476209	2.864992	−0.506556
H	1.134666	2.499819	0.111084
H	0.681129	1.958288	−1.509552
C	1.860880	−0.321927	1.056263
H	2.462568	−1.232624	1.013196
H	2.507178	0.525579	0.828889
H	1.474428	−0.215720	2.069109
O	1.228495	−0.424993	−1.278834
H	1.825699	−1.173877	−1.357264

Table S40: M06-2X optimized geometry of *cis*-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.943194	0.592819	−0.037696
C	−1.742075	−0.550538	−0.538229
C	−0.896463	−1.808488	−0.481496
C	0.213922	−1.460352	0.517658
C	0.438992	0.056592	0.357252
C	1.447102	0.368164	−0.761267
C	2.871469	−0.087676	−0.464080
H	2.944242	−1.164793	−0.317730
H	3.532624	0.173988	−1.289033
H	3.263492	0.407215	0.425440
H	1.094499	−0.086294	−1.691694
H	1.457219	1.447043	−0.914578
O	0.837832	0.693453	1.557885
H	1.636536	0.269748	1.882099
H	−0.122573	−1.644851	1.535227
H	1.119782	−2.038608	0.346598
H	−1.466150	−2.688877	−0.189171
H	−0.481476	−1.995377	−1.475440
S	−2.289460	0.075823	1.076044
H	−2.441741	−0.408489	−1.351449
C	−1.059712	1.976808	−0.619535
H	−0.556094	2.040274	−1.585176
H	−2.107178	2.234310	−0.758972
H	−0.610067	2.706002	0.054571

Table S41: M06-2X optimized geometry of *cis*-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.405238	0.098892	0.698443
C	−0.696157	0.622419	−0.241158
C	−1.380355	−0.537409	−0.844216
C	−0.719132	−1.820407	−0.381353
C	0.086797	−1.406794	0.857834
H	0.996165	−1.993189	0.982735
H	−0.511466	−1.536968	1.757372
H	−0.065809	−2.176897	−1.179624
H	−1.442362	−2.606107	−0.169844
S	−2.379269	0.314892	0.422932
H	−1.786392	−0.470758	−1.845291
C	−0.499963	1.934406	−0.949195
H	−1.392742	2.198889	−1.511754
H	−0.301083	2.722275	−0.222384
H	0.345863	1.883838	−1.636688
O	0.411488	0.786604	1.932965
H	−0.479994	0.729841	2.295594
C	1.798219	0.341181	0.115690
C	2.086306	−0.373300	−1.198855
H	1.337993	−0.148386	−1.961184
H	3.056451	−0.070491	−1.589867
H	2.111071	−1.454997	−1.067521
H	1.933028	1.417909	0.005388
H	2.509906	0.018608	0.877490

Table S42: M06-2X optimized geometry of *trans*-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	−0.466466	−0.007869	0.137146
C	0.891424	0.650555	−0.138306
C	1.919242	−0.410393	−0.049514
C	1.251220	−1.724776	0.294976
C	−0.216246	−1.507926	−0.096105
H	−0.898635	−2.114466	0.499119
H	−0.375508	−1.753851	−1.144394
H	1.338089	−1.873273	1.373173
H	1.703136	−2.578996	−0.205649
S	1.632434	0.202973	−1.741541
H	2.897296	−0.181034	0.351581
C	1.121697	2.049201	0.364175
H	2.154380	2.343489	0.186947
H	0.474539	2.758864	−0.151311
H	0.905327	2.097065	1.430517
C	−1.606113	0.574290	−0.688726
C	−2.954438	−0.078219	−0.405397
H	−2.930616	−1.148356	−0.614502
H	−3.258110	0.061122	0.633941
H	−3.735185	0.361523	−1.023958
H	−1.665089	1.644672	−0.480788
H	−1.351110	0.458963	−1.743518
O	−0.673880	0.231510	1.532417
H	−1.458996	−0.249566	1.806477

Table S43: M06-2X optimized geometry of *cis*-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.470402	−0.222336	0.057678
C	0.005181	−1.392204	−0.719834
C	1.451705	−1.170942	−1.123441
C	1.946811	−0.100665	−0.143308
C	0.705536	0.757039	0.167501
C	0.561778	1.879283	−0.860275
H	1.449668	2.513947	−0.830233
H	0.469576	1.481602	−1.872382
H	−0.308192	2.495796	−0.643265
O	0.714189	1.302829	1.474304
H	1.396809	1.977593	1.521412
H	2.284814	−0.558405	0.783035
H	2.760314	0.497942	−0.552746
H	2.042894	−2.084394	−1.088019
H	1.474534	−0.799496	−2.151349
S	−0.253205	−1.739177	1.043177
H	−0.664144	−1.910391	−1.393991
C	−1.858992	0.367574	−0.067940
C	−3.007873	−0.629136	−0.024740
H	−3.078233	−1.106849	0.949489
H	−3.949278	−0.121486	−0.231645
H	−2.881514	−1.416143	−0.769285
H	−1.976476	1.107234	0.727406
H	−1.898908	0.915402	−1.013190

Table S44: M06-2X optimized geometry of *cis*-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−1.855618	0.006910	0.574472
C	−0.380790	−0.316772	0.440674
C	0.123092	−1.577106	−0.140461
C	1.377541	−1.293610	−0.944116
C	1.886962	0.036129	−0.380180
C	0.627776	0.797113	0.091852
C	0.105023	1.702207	−1.013445
H	−0.815868	2.196959	−0.709643
H	0.854235	2.467403	−1.211742
H	−0.073404	1.139517	−1.930069
O	0.875637	1.649076	1.189937
H	1.150925	1.091973	1.927072
H	2.534033	−0.140712	0.476431
H	2.449230	0.616786	−1.109042
H	2.111754	−2.094565	−0.879035
H	1.091109	−1.188315	−1.994040
S	0.316437	−1.491651	1.670908
H	−0.566558	−2.341077	−0.473982
H	−2.297222	−0.691493	1.283133
H	−1.943414	1.000412	1.019910
C	−2.638778	−0.068885	−0.736718
H	−2.289602	0.649255	−1.474732
H	−2.562537	−1.064469	−1.174832
H	−3.694145	0.130221	−0.552906

Table S45: M06-2X optimized geometry of *trans*-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	0.676163	0.892131	0.113874
C	1.968099	0.123477	−0.203446
C	1.516922	−1.036892	−1.097957
C	0.122551	−1.356739	−0.599301
C	−0.418696	−0.186748	0.130316
C	−1.855628	0.282257	0.059923
H	−1.903875	1.047107	−0.715742
C	−2.877655	−0.810024	−0.221411
H	−2.817014	−1.607557	0.517659
H	−3.884774	−0.396500	−0.197350
H	−2.726427	−1.246631	−1.208745
H	−2.097076	0.776602	1.003833
S	−0.025430	−1.610370	1.200699
H	−0.528573	−1.983809	−1.191975
H	1.436158	−0.707506	−2.135706
H	2.188739	−1.892318	−1.059940
H	2.689678	0.778110	−0.692395
H	2.417075	−0.250317	0.714021
C	0.750061	1.726028	1.377936
H	0.928592	1.089841	2.243970
H	1.568122	2.446586	1.308111
H	−0.178970	2.276859	1.523456
O	0.328838	1.712309	−1.006657
H	0.983369	2.412360	−1.077651

Table S46: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
130.2	0.7
186.7	1.3
213.5	0.8
228.8	78.7
242.1	21.9
267.6	0.4
310.5	0.6
362.7	2.0
380.6	3.0
422.6	1.7
482.3	13.4
534.7	13.5
587.7	5.9
661.5	1.7
691.4	3.9
813.3	3.5
853.7	6.7
894.6	15.8
944.1	6.5
949.4	2.4
955.5	9.8
994.9	1.5
1011.5	6.2
1046.2	7.5
1088.0	13.9
1102.1	62.0
1127.5	12.2
1169.4	17.1
1212.0	12.5
1227.1	37.9
1242.5	26.5
1261.0	27.6
1306.3	7.0
1333.5	4.0
1343.7	11.8
1402.4	18.5
1405.4	6.1
1412.6	8.5
1474.4	4.3
1484.2	7.2
1490.4	6.6
1496.1	10.6
1499.9	3.2
1507.6	8.4
1522.4	5.5
3055.0	12.1
3070.6	15.3
3072.5	21.2
3092.4	25.8
3118.7	16.5
3122.5	22.8
3139.4	12.4
3147.7	10.8
3152.2	11.2
3156.7	10.8
3178.1	20.1
3872.3	32.3

Table S47: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
112.7	3.0
198.3	0.1
213.9	1.1
232.7	1.3
266.6	0.8
305.9	0.6
354.6	3.9
373.1	2.9
417.4	29.4
441.1	49.9
483.1	33.2
539.4	14.6
594.6	5.2
664.7	2.6
686.8	4.3
810.2	0.6
846.3	5.7
896.4	13.7
944.0	8.3
951.2	4.7
963.1	5.4
995.3	14.1
1014.5	8.6
1046.7	28.2
1084.1	13.5
1117.4	6.8
1126.0	24.0
1170.9	37.1
1183.9	3.0
1228.1	48.9
1246.8	11.2
1295.8	19.2
1314.7	1.7
1336.5	3.0
1352.3	0.7
1389.9	40.7
1410.1	11.6
1429.0	34.3
1476.6	2.9
1482.9	7.7
1487.5	9.9
1494.8	10.0
1500.1	3.1
1509.5	4.0
1523.5	5.0
3066.1	8.4
3068.5	15.1
3074.5	22.4
3098.1	15.3
3120.0	19.0
3137.2	11.9
3141.9	11.5
3145.8	14.6
3151.3	20.2
3156.4	8.1
3182.4	19.1
3843.0	32.8

Table S48: M06-2X/cc-pVTZ Frequencies and IR Intensities of trans-2,3-epoxy-1,2-dimethylcyclopentan-1-ol

Frequency	IR Intensity
118.5	2.1
183.0	0.4
223.6	4.4
242.5	2.1
264.0	0.2
271.0	28.1
282.6	71.8
353.5	2.0
381.6	7.6
425.5	1.2
481.3	14.5
513.9	1.9
600.0	2.4
654.6	1.2
701.7	1.9
814.6	3.6
855.2	4.5
888.5	8.2
937.2	3.7
952.1	20.9
960.2	13.1
992.7	2.2
1016.7	6.0
1042.3	6.2
1091.6	5.6
1096.4	82.5
1125.4	12.5
1165.5	1.4
1209.5	5.9
1231.1	68.3
1241.5	15.3
1260.0	3.9
1304.4	5.6
1339.6	5.7
1352.3	3.5
1402.3	3.2
1405.7	17.5
1416.9	23.6
1473.0	2.5
1483.4	5.4
1487.5	14.2
1491.4	5.2
1495.6	6.1
1506.2	2.0
1522.0	7.2
3053.3	16.2
3068.9	16.8
3082.8	24.6
3093.6	25.0
3123.0	14.5
3125.9	12.1
3137.7	11.7
3143.5	6.4
3147.8	23.2
3164.0	5.9
3186.1	19.6
3874.1	32.6

Table S49: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
77.2	0.5
124.9	1.1
170.6	12.8
196.3	72.3
204.3	4.1
224.6	6.1
274.7	18.9
286.2	3.0
322.3	1.5
356.6	1.3
392.2	3.1
423.9	4.3
484.4	10.2
546.0	12.1
591.4	4.8
662.6	1.8
708.2	2.4
794.0	1.0
804.5	5.3
854.5	7.0
894.8	15.3
945.3	1.3
951.3	16.2
981.9	7.0
1004.2	17.4
1031.0	0.7
1038.2	13.6
1052.8	19.7
1093.1	16.5
1105.5	20.7
1125.2	16.9
1165.7	15.2
1195.9	9.1
1235.0	56.0
1239.2	6.9
1249.3	22.6
1301.7	1.1
1318.9	2.6
1334.4	4.7
1346.3	10.7
1367.0	4.9
1400.3	9.2
1409.8	5.5
1422.9	6.2
1475.6	1.1
1483.5	11.6
1484.5	7.7
1495.6	9.6
1498.5	3.8
1506.6	6.3
1517.0	8.6
1520.2	6.7
3058.7	10.6
3067.2	19.6
3071.7	15.4
3073.9	24.1
3103.3	20.2
3107.0	9.3
3119.7	15.4
3134.9	23.9
3139.3	24.6
3143.4	11.8
3155.5	13.0
3157.6	12.3
3180.1	21.3
3881.1	31.9

Table S50: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
130.0	1.6
141.6	1.3
199.1	0.3
224.1	0.3
242.5	0.6
257.5	1.7
263.1	1.5
310.7	0.9
373.2	4.8
402.0	4.7
437.1	35.2
458.0	27.0
485.3	47.9
533.2	10.4
616.2	5.1
650.7	0.8
690.9	5.7
790.1	0.4
821.3	0.9
842.8	5.4
895.2	12.1
941.0	3.3
947.2	23.6
976.9	14.0
1006.2	1.1
1025.6	12.2
1054.0	23.1
1075.0	17.4
1087.8	19.0
1122.8	3.8
1130.5	33.3
1171.0	20.4
1184.3	9.8
1203.5	37.4
1246.4	1.2
1271.9	3.6
1294.6	9.5
1326.3	2.7
1336.1	6.9
1345.4	2.8
1383.3	20.5
1409.8	11.9
1411.8	30.0
1420.5	7.2
1475.8	3.3
1482.5	11.0
1493.7	12.4
1497.4	3.6
1501.2	2.1
1507.5	10.7
1517.7	5.7
1522.7	7.2
3062.6	9.8
3066.9	11.2
3072.2	23.1
3080.5	26.1
3096.9	17.0
3105.3	2.4
3119.6	15.0
3130.9	32.6
3135.5	8.7
3140.3	34.2
3143.2	11.7
3155.3	9.6
3178.6	18.6
3840.7	33.4

Table S51: Frequencies and IR Intensities of trans-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol.

Frequency	IR Intensity
97.8	0.2
117.7	2.3
169.5	1.1
192.0	1.0
239.3	11.7
246.1	4.5
269.5	64.4
276.5	28.9
303.1	4.2
362.5	2.0
404.1	2.9
437.0	3.6
489.5	11.5
521.8	2.3
588.1	1.7
677.8	0.6
704.6	2.2
789.4	4.1
826.5	2.9
851.3	6.7
895.4	9.4
946.2	5.1
967.7	20.0
983.6	7.4
991.7	23.0
1026.1	26.3
1033.8	2.5
1048.2	2.4
1092.9	4.6
1101.1	38.4
1126.4	17.8
1167.1	1.9
1204.8	2.6
1226.8	66.9
1240.4	4.6
1249.1	12.2
1302.7	5.6
1319.9	5.1
1336.8	7.6
1351.2	2.3
1361.6	3.3
1405.0	15.9
1410.5	3.0
1428.6	17.3
1474.3	2.2
1482.7	8.5
1486.2	5.2
1492.3	3.7
1494.0	7.1
1505.6	8.1
1513.9	5.7
1522.8	8.0
3057.0	13.1
3064.4	16.3
3070.1	21.8
3081.9	26.6
3090.9	20.0
3102.3	2.3
3124.2	8.1
3125.5	31.2
3138.5	6.5
3139.5	29.0
3141.8	19.9
3163.6	6.0
3185.8	20.7
3880.2	29.3

Table S52: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
84.6	0.2
116.0	1.0
185.8	0.5
199.4	5.1
221.0	83.7
233.6	8.6
276.4	2.7
303.6	1.6
319.0	1.0
364.0	1.8
406.2	3.1
442.7	3.3
487.5	13.5
556.1	4.1
599.6	15.4
650.7	2.0
697.1	2.0
775.3	2.6
815.9	3.9
870.1	11.0
922.7	5.0
947.6	2.1
957.6	15.3
968.4	8.2
981.7	10.7
1016.4	7.0
1026.4	19.3
1058.6	4.8
1090.7	13.2
1112.9	37.4
1123.3	5.4
1168.0	25.1
1211.5	10.7
1219.0	39.5
1239.6	13.0
1244.8	30.8
1293.9	8.9
1310.5	1.2
1332.5	6.7
1342.1	12.5
1371.8	1.6
1405.4	18.2
1411.3	0.7
1415.3	7.4
1478.4	6.4
1484.2	0.5
1494.3	8.6
1498.2	10.2
1500.3	7.4
1504.2	1.2
1510.0	11.1
1515.8	6.8
3053.4	11.6
3068.6	17.2
3073.7	27.4
3074.1	10.7
3092.6	25.3
3115.7	0.5
3119.0	16.3
3121.3	32.4
3135.8	24.6
3143.1	17.4
3148.3	19.1
3152.5	10.7
3179.4	20.1
3872.4	32.4

Table S53: Frequencies and IR Intensities of cis-2-ethyl-2,3-epoxy-1-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
97.5	1.4
104.3	1.5
172.2	0.6
201.6	0.2
229.0	2.0
274.2	0.3
300.4	1.7
318.1	0.7
359.5	2.2
398.9	16.1
422.9	62.8
443.9	11.3
486.2	30.6
558.8	5.9
605.2	11.9
654.4	3.9
693.4	2.9
779.3	2.8
815.4	1.3
864.9	7.8
925.8	1.4
949.4	2.3
957.6	19.3
968.5	4.5
980.2	15.3
1018.6	25.8
1027.9	14.5
1059.8	22.9
1091.6	5.9
1113.7	8.0
1126.6	12.1
1173.3	31.3
1182.2	3.3
1226.1	47.0
1241.3	15.3
1268.0	1.4
1300.4	15.2
1316.8	8.6
1336.2	2.2
1351.3	0.2
1373.3	6.2
1393.5	30.1
1415.1	6.1
1428.3	36.8
1480.5	9.1
1481.8	3.1
1491.2	4.0
1498.9	9.5
1500.5	8.4
1506.3	0.8
1511.9	6.6
1517.3	4.9
3064.5	7.6
3067.1	10.4
3071.8	23.3
3073.7	24.2
3099.1	15.2
3111.6	2.5
3119.6	19.8
3137.1	23.2
3141.5	17.7
3144.6	14.8
3147.7	33.6
3151.7	6.6
3178.3	19.1
3843.0	33.6

Table S54: Frequencies and IR Intensities of trans-2-ethyl-2,3-epoxy-1-methylcyclopentan-1-ol

Frequency	IR Intensity
42.0	0.0
120.9	1.7
173.1	1.4
219.7	1.8
229.4	3.8
260.0	8.3
261.8	80.6
275.5	6.0
307.4	1.9
377.2	7.5
396.5	3.4
433.2	1.6
483.1	14.4
554.8	5.3
596.0	2.5
647.0	2.8
705.3	0.2
778.9	3.3
819.4	1.8
872.6	5.7
910.5	1.8
940.9	4.0
958.2	7.2
971.1	29.3
999.2	3.1
1008.6	20.2
1028.9	15.8
1064.6	12.0
1091.8	20.5
1104.8	38.7
1128.8	4.5
1164.2	1.6
1207.4	5.4
1226.7	49.7
1239.8	19.4
1244.4	12.0
1292.5	5.1
1314.3	8.1
1336.1	7.6
1351.8	3.1
1368.6	1.3
1404.5	8.6
1412.9	1.3
1421.7	24.3
1472.6	2.8
1485.7	4.3
1490.9	4.4
1496.9	3.3
1497.3	14.7
1500.9	6.7
1507.2	1.3
1519.4	6.2
3053.9	14.9
3063.2	17.4
3070.6	29.4
3080.8	24.3
3092.5	25.0
3104.9	12.5
3123.6	10.2
3124.7	16.3
3133.1	31.9
3144.2	8.0
3149.5	20.3
3172.0	8.5
3181.8	18.7
3870.4	31.6

Table S55: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
133.3	0.6
180.0	89.5
198.2	9.7
217.7	4.0
243.0	1.3
274.1	1.0
324.1	0.6
367.0	2.1
382.7	1.7
426.6	4.9
482.2	8.1
522.7	17.5
587.4	4.1
655.5	1.7
672.1	2.3
813.0	1.9
855.1	0.6
874.1	26.0
931.0	5.5
948.6	7.3
956.7	13.6
976.8	5.8
1005.0	8.4
1018.3	34.4
1054.4	24.4
1091.9	19.1
1094.6	15.6
1128.4	32.2
1154.5	23.3
1166.5	19.3
1211.1	18.7
1241.4	25.8
1246.7	17.1
1297.2	16.4
1317.6	21.6
1339.1	1.1
1354.4	10.3
1403.8	23.0
1412.0	6.4
1419.3	4.4
1470.0	5.7
1482.4	5.7
1489.6	9.4
1492.9	7.1
1500.4	3.9
1504.1	6.7
1518.4	1.0
3054.9	13.1
3060.3	20.9
3070.9	28.3
3090.5	31.0
3115.6	19.9
3122.2	24.7
3129.6	14.2
3133.7	15.5
3146.9	15.9
3154.3	10.7
3186.3	16.6
3544.3	2.3
3873.7	29.3

Table S56: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
117.6	2.1
214.0	0.0
220.3	0.2
230.2	1.0
272.8	0.8
320.0	0.9
354.9	5.3
377.0	1.8
425.4	7.7
454.8	51.3
484.5	44.2
528.0	16.8
594.9	4.1
660.6	8.3
668.9	1.1
813.2	0.2
847.1	0.3
878.9	15.4
931.6	9.8
946.3	11.5
961.6	8.7
981.3	1.7
1008.0	11.9
1024.1	56.7
1055.0	24.8
1091.3	5.0
1111.0	9.0
1133.8	21.4
1139.1	10.8
1182.0	1.4
1204.1	18.5
1234.2	84.9
1252.6	0.5
1305.7	10.7
1338.7	4.0
1353.0	0.5
1360.2	6.4
1394.5	36.0
1415.1	9.6
1431.7	45.5
1473.6	3.9
1483.3	7.4
1488.5	8.0
1491.0	8.6
1501.7	2.1
1504.1	6.4
1519.8	1.2
3057.2	19.6
3064.4	11.6
3071.3	29.2
3097.9	17.4
3115.3	21.4
3125.9	13.3
3133.4	13.2
3139.9	17.9
3145.2	18.7
3150.5	16.6
3188.6	16.2
3540.2	2.6
3831.2	30.5

Table S57: M06-2X/cc-pVTZ Frequencies and IR Intensities of trans-2,3- aziridine-1,2-dimethylcyclopentan-1-ol

Frequency	IR Intensity
125.1	1.2
200.1	0.3
228.3	7.4
245.1	3.6
255.9	87.0
261.0	0.0
286.9	7.9
352.2	1.3
385.6	8.3
432.7	0.4
476.0	17.0
502.0	1.6
600.7	4.8
649.0	0.1
684.7	0.2
816.3	2.7
854.4	1.8
873.8	15.4
925.7	6.8
946.7	15.4
957.9	10.2
975.2	18.9
1005.1	10.5
1024.8	44.7
1049.4	36.0
1093.7	13.0
1099.4	15.1
1130.9	9.7
1145.3	6.2
1170.7	5.0
1210.3	6.9
1239.4	18.1
1247.6	72.0
1298.5	15.4
1317.4	12.0
1348.2	1.7
1359.1	2.9
1401.4	12.2
1409.7	11.8
1424.0	13.0
1472.8	2.4
1479.3	9.0
1484.8	8.7
1492.5	2.6
1495.1	5.1
1505.1	3.2
1514.2	3.7
3052.6	19.1
3056.7	25.4
3080.0	29.4
3090.1	31.9
3117.8	23.1
3121.5	14.5
3123.3	13.8
3143.8	3.6
3148.3	23.8
3153.3	6.4
3193.3	16.1
3541.9	2.4
3876.5	31.0

Table S58: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-aziridine-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
69.1	3.0
125.2	23.4
144.9	75.2
186.8	5.1
210.8	1.2
225.5	1.8
273.2	9.3
297.7	1.2
333.5	0.6
362.9	0.8
389.1	1.9
429.1	7.8
485.5	3.6
536.1	16.4
589.2	2.7
651.1	2.2
696.0	1.7
792.5	0.6
803.1	2.8
855.6	1.5
873.7	24.4
931.9	10.6
953.7	3.6
977.8	13.1
982.5	45.4
1012.2	13.1
1026.7	1.9
1051.9	34.9
1054.4	18.8
1096.2	3.3
1099.8	11.1
1127.2	31.8
1153.0	19.4
1163.1	3.3
1194.4	9.1
1235.1	29.4
1257.8	11.5
1282.1	33.7
1305.2	0.2
1323.2	5.9
1344.0	1.0
1357.9	8.5
1373.2	8.6
1403.7	8.6
1414.3	5.3
1424.0	5.0
1472.1	4.2
1481.0	9.7
1484.4	9.2
1494.4	6.9
1500.1	2.1
1508.2	5.4
1513.8	5.4
1515.5	8.4
3057.2	9.2
3060.6	22.6
3067.1	21.4
3071.5	32.6
3102.8	23.2
3106.7	10.4
3117.2	18.8
3128.5	14.6
3133.6	25.8
3137.7	5.4
3141.5	38.7
3155.8	14.7
3187.1	17.3
3544.4	2.2
3883.7	30.5

Table S59: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-aziridine-1-ethyl-2-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
77.6	0.6
117.4	1.1
185.2	0.9
215.8	0.3
222.2	0.4
243.4	1.2
290.4	2.0
326.1	1.0
355.1	1.8
385.3	3.1
429.5	6.3
468.6	36.8
490.0	55.1
540.5	19.2
596.4	3.0
655.1	8.3
694.5	1.3
795.5	0.4
804.7	0.4
847.2	1.2
877.9	13.3
933.3	15.2
953.3	6.6
983.0	57.5
987.6	6.4
1019.1	8.6
1035.2	7.1
1052.8	23.2
1053.7	24.0
1097.8	7.2
1105.3	5.7
1133.5	16.6
1139.9	10.8
1173.8	4.9
1194.6	6.7
1224.1	74.3
1251.9	2.3
1294.6	4.3
1322.4	0.9
1340.3	10.8
1344.7	1.8
1362.5	4.2
1371.0	20.4
1411.2	7.7
1415.1	11.7
1430.4	37.3
1474.0	1.9
1480.4	11.6
1486.1	9.6
1492.0	5.3
1499.2	1.5
1508.4	9.0
1512.5	5.5
1514.3	6.6
3053.1	17.5
3057.4	21.1
3070.8	30.3
3074.7	22.5
3100.5	14.7
3106.7	11.0
3118.1	22.2
3125.5	14.4
3135.8	6.0
3138.9	43.9
3153.2	5.4
3159.5	24.6
3188.5	17.0
3537.7	2.6
3832.1	34.0

Table S60: M06-2X/cc-pVTZ Frequencies and IR Intensities of trans-2,3-aziridine-1-ethyl-2-methylcyclopentan-1-ol

Frequency	IR Intensity
99.6	0.1
123.0	1.3
175.1	1.4
201.8	0.2
242.9	13.8
246.4	1.6
277.6	73.2
285.4	18.4
305.3	7.1
362.0	2.0
409.4	3.3
440.9	2.1
486.0	15.0
509.1	3.1
586.9	3.9
669.5	0.4
692.3	0.3
790.2	3.4
829.4	2.6
850.8	2.0
875.5	16.1
933.3	11.9
963.2	5.7
975.1	15.0
990.4	8.7
1004.5	80.7
1025.3	16.7
1041.3	1.8
1052.9	18.6
1096.0	2.1
1103.0	6.4
1130.2	11.9
1143.3	4.4
1173.4	2.6
1203.5	3.3
1233.4	55.3
1245.8	14.4
1284.3	38.0
1313.0	10.9
1324.2	0.6
1343.8	1.0
1360.0	2.5
1368.2	4.0
1407.1	14.7
1412.0	2.3
1431.6	10.5
1475.3	2.1
1480.8	6.7
1484.4	8.9
1489.9	1.6
1493.6	3.9
1506.2	8.0
1512.4	6.6
1514.6	4.2
3056.4	18.4
3057.1	13.6
3063.6	31.7
3079.7	32.1
3089.4	26.5
3102.3	1.3
3119.0	23.1
3121.9	10.2
3125.5	28.7
3137.7	25.8
3142.3	19.0
3152.3	6.0
3193.0	16.8
3539.9	2.5
3882.6	28.1

Table S61: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-aziridine-1-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
88.1	0.2
118.0	0.3
187.9	3.6
207.8	31.0
214.6	64.0
243.1	0.9
279.9	4.0
306.5	0.8
336.7	0.6
370.1	1.5
416.7	4.3
442.0	4.6
486.2	11.8
545.1	5.4
597.2	8.9
647.1	1.8
678.9	3.4
771.2	3.2
816.7	3.7
868.4	3.6
885.0	20.8
944.2	2.9
948.7	39.0
966.8	6.8
979.4	1.9
1008.8	2.4
1020.6	2.2
1023.9	32.5
1076.3	18.6
1092.5	13.4
1109.0	11.9
1119.7	1.8
1150.9	68.1
1161.2	12.5
1211.2	17.6
1239.7	19.3
1243.9	24.5
1262.2	9.2
1312.2	8.9
1324.9	16.2
1337.0	2.0
1352.0	12.1
1372.7	2.4
1405.9	18.8
1413.0	5.5
1424.6	10.2
1466.7	4.8
1480.6	2.8
1489.7	3.0
1494.6	9.6
1498.8	6.8
1504.9	3.4
1509.7	4.9
1515.0	8.1
3053.3	13.5
3061.1	18.4
3068.9	23.7
3069.7	28.5
3089.9	29.3
3095.3	8.5
3114.5	20.7
3120.5	33.7
3132.7	26.4
3143.3	16.6
3153.3	17.5
3154.0	10.7
3188.5	16.2
3546.3	2.2
3872.5	29.2

Table S62: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-aziridine-1-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
98.4	0.8
108.1	0.9
173.8	0.5
211.3	0.3
242.2	1.0
276.9	0.3
301.0	2.5
338.3	0.4
364.5	2.1
410.1	3.2
440.3	2.3
467.9	24.0
498.5	83.6
547.9	5.9
603.9	6.2
652.3	8.4
676.9	4.0
775.1	3.3
817.1	1.2
863.9	2.0
890.4	11.6
940.9	21.2
948.5	17.3
968.8	11.5
983.9	2.2
1012.2	3.3
1022.2	21.2
1030.6	39.0
1073.9	20.7
1097.1	3.8
1109.6	12.1
1124.5	5.0
1141.4	14.1
1178.2	3.7
1202.1	20.4
1234.0	86.5
1249.6	0.7
1273.2	0.4
1315.0	11.5
1336.2	7.6
1350.3	1.5
1364.9	12.5
1374.3	5.0
1400.9	25.3
1415.4	6.6
1433.4	51.9
1472.3	4.6
1482.3	3.6
1487.5	5.2
1491.0	8.8
1500.1	7.0
1505.3	3.0
1511.5	3.3
1516.3	3.7
3053.6	21.1
3064.6	9.4
3069.6	25.3
3070.9	27.6
3089.7	9.7
3098.9	17.9
3115.2	23.4
3134.0	25.6
3141.6	19.2
3144.5	14.0
3147.8	24.4
3158.9	13.4
3185.7	16.2
3539.0	2.7
3826.3	31.7

Table S63: M06-2X/cc-pVTZ Frequencies and IR Intensities of trans-2-ethyl-2,3-aziridine-1-methylcyclopentan-1-ol

Frequency	IR Intensity
43.5	0.1
123.7	1.0
180.8	0.8
232.4	0.4
236.9	4.0
262.6	0.5
268.4	1.6
297.1	86.5
310.5	4.2
380.9	10.8
402.5	4.7
439.8	0.2
476.8	16.2
541.6	3.7
597.3	4.6
642.3	0.9
690.1	0.8
774.4	3.6
819.2	3.1
870.3	2.8
885.0	13.4
931.1	13.2
947.2	26.4
965.3	28.4
988.9	1.1
1004.8	5.1
1023.9	27.4
1031.8	22.7
1077.4	14.2
1096.4	22.9
1105.6	13.8
1126.3	3.1
1138.9	1.3
1169.4	5.7
1207.9	7.1
1238.7	7.8
1244.7	87.2
1266.2	1.0
1313.9	12.0
1324.3	15.2
1349.1	4.6
1357.6	2.6
1370.6	3.5
1401.4	14.9
1414.8	8.7
1430.3	12.3
1468.5	2.5
1479.6	6.5
1482.3	3.4
1493.3	3.8
1495.7	4.0
1499.3	4.9
1504.5	4.3
1516.6	4.9
3046.2	26.4
3053.2	19.1
3068.9	25.9
3078.5	28.9
3083.3	22.9
3090.1	34.1
3121.5	13.8
3122.2	17.9
3130.1	33.9
3145.8	3.8
3150.3	23.0
3179.1	6.6
3188.4	15.6
3542.3	2.5
3871.3	29.5

Table S64: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
119.3	0.0
208.9	2.2
213.7	1.1
236.8	7.6
260.1	80.6
276.8	1.4
308.7	0.9
324.0	6.8
354.0	0.0
383.1	0.8
429.2	3.9
481.9	10.1
560.0	1.5
596.4	0.2
607.9	0.9
652.2	1.4
715.3	1.7
765.7	1.7
837.9	4.2
894.3	8.0
921.9	9.3
945.2	8.4
957.6	1.0
978.7	0.3
989.4	7.0
1014.9	8.3
1053.2	4.3
1086.7	19.0
1105.2	25.8
1141.3	21.3
1177.2	33.3
1204.2	7.9
1236.0	53.3
1238.4	6.6
1262.6	4.2
1324.2	18.6
1330.3	16.0
1368.3	2.3
1396.7	27.2
1403.6	8.2
1412.9	4.5
1488.2	2.3
1489.8	2.8
1496.4	9.1
1499.4	12.1
1510.0	4.7
1516.3	1.7
2429.9	78.0
3053.4	15.0
3055.3	27.5
3059.3	34.6
3081.8	13.0
3115.2	19.1
3117.7	14.6
3122.8	21.6
3129.4	26.1
3143.6	11.7
3151.9	12.7
3196.7	5.4
3871.0	30.6

Table S65: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
126.2	1.8
209.0	0.5
217.1	0.1
236.5	0.2
266.4	1.2
308.1	0.3
316.5	0.5
347.4	8.9
367.7	53.8
387.4	21.4
428.6	6.2
479.2	12.3
560.3	3.3
595.7	0.2
608.4	5.9
642.6	1.6
710.6	2.0
759.6	1.0
833.6	0.5
885.5	8.2
925.9	1.6
948.8	1.6
963.2	4.0
979.5	0.0
990.3	6.4
1016.5	44.7
1051.9	3.7
1089.3	8.5
1101.2	9.3
1142.9	29.4
1168.4	6.8
1210.6	4.5
1238.8	68.7
1245.2	16.6
1264.2	4.6
1324.8	3.0
1340.5	7.8
1379.8	45.8
1384.6	18.7
1414.3	4.1
1418.4	32.9
1482.9	2.1
1490.1	1.7
1494.6	9.1
1497.9	14.2
1509.0	6.2
1517.2	1.0
2441.7	67.1
3055.6	24.7
3062.0	20.9
3069.7	18.9
3078.3	10.5
3119.2	21.2
3119.4	12.3
3135.3	19.0
3142.9	10.2
3144.5	20.9
3157.1	13.2
3195.7	4.6
3837.3	19.6

Table S66: M06-2X/cc-pVTZ Frequencies and IR Intensities of trans-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol

Frequency	IR Intensity
119.7	0.7
196.6	0.1
218.3	3.2
236.3	22.3
243.2	3.9
256.2	66.5
293.3	2.1
318.8	1.1
330.2	4.4
390.3	6.1
410.3	2.4
457.5	2.2
561.9	2.6
608.8	1.1
611.1	3.5
654.0	12.3
724.3	2.2
784.1	3.3
826.6	6.3
893.9	7.8
911.4	4.8
945.6	0.7
955.6	22.8
980.7	12.6
988.3	2.3
1019.8	6.1
1056.1	3.9
1081.5	62.9
1096.2	0.4
1140.4	2.1
1179.4	30.1
1207.1	5.2
1227.5	0.4
1238.9	15.5
1258.4	33.9
1323.6	4.7
1342.5	4.1
1367.5	7.6
1395.7	10.6
1408.9	17.7
1412.5	14.3
1484.2	1.2
1486.0	9.2
1493.4	1.6
1498.9	4.6
1499.8	6.4
1504.6	8.1
2435.5	71.9
3054.6	18.4
3062.9	26.5
3075.8	27.9
3076.6	13.1
3118.9	14.7
3123.8	23.4
3129.4	19.0
3129.5	15.8
3143.0	8.2
3148.2	14.1
3199.9	4.4
3871.0	30.1

Table S67: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
65.8	0.1
120.6	0.0
179.0	0.6
211.2	63.0
219.7	1.0
229.2	13.8
277.5	11.0
290.7	10.4
316.1	2.4
341.7	5.7
352.0	2.7
372.7	0.5
428.3	4.7
507.3	7.4
559.9	1.4
595.1	0.6
635.3	1.5
664.2	1.4
728.0	1.8
744.5	0.8
796.7	1.7
841.4	4.4
902.8	8.1
925.6	11.1
944.2	5.4
961.1	4.9
985.5	6.9
1013.1	14.7
1020.8	2.5
1046.2	17.1
1061.6	8.2
1086.8	8.2
1109.3	15.3
1141.0	18.9
1176.5	14.7
1192.1	9.2
1231.9	44.4
1235.2	10.3
1267.2	3.7
1309.2	11.9
1316.7	21.2
1332.9	0.8
1359.9	9.3
1374.7	0.6
1399.5	20.6
1412.1	4.1
1421.7	6.4
1479.8	2.9
1496.3	9.8
1497.5	6.8
1504.3	5.8
1507.3	5.0
1510.3	3.0
1519.4	12.6
2434.1	79.0
3055.1	24.8
3058.0	18.0
3062.6	18.4
3066.4	30.9
3088.0	10.1
3112.2	11.8
3116.5	16.1
3121.0	12.2
3130.7	15.3
3136.3	29.6
3142.9	15.2
3148.0	29.6
3195.6	5.7
3878.5	29.8

Table S68: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
129.9	0.9
154.3	0.2
220.4	0.1
227.6	0.1
233.9	0.4
257.5	0.4
290.3	0.1
315.0	0.8
328.8	2.9
357.9	6.0
373.8	70.7
415.3	4.2
446.8	11.4
476.5	6.2
564.2	2.9
599.3	2.6
602.3	1.8
652.1	2.4
711.6	1.8
747.9	2.5
798.7	2.8
835.9	0.4
891.4	8.5
928.7	4.8
938.3	8.5
961.4	3.4
983.6	10.2
1009.6	7.3
1038.2	17.1
1057.3	6.2
1075.8	28.5
1088.2	10.6
1111.6	14.5
1143.7	20.0
1173.5	8.9
1196.0	23.3
1223.3	24.6
1241.6	7.2
1252.1	6.1
1308.8	3.4
1324.9	0.9
1330.2	2.4
1372.1	41.1
1388.4	12.1
1396.6	31.8
1414.3	12.2
1419.3	2.8
1485.7	0.3
1492.1	9.7
1495.2	14.4
1502.9	2.9
1507.5	15.8
1512.2	2.6
1524.4	3.5
2441.3	65.4
3056.3	22.0
3063.4	12.2
3075.4	15.4
3079.3	14.0
3082.4	32.9
3109.4	1.9
3118.4	19.2
3119.5	14.0
3129.1	23.8
3133.1	37.9
3139.9	19.1
3141.2	12.6
3192.9	4.1
3835.9	20.3

Table S69: M06-2X/cc-pVTZ Frequencies and IR Intensities of trans-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol

Frequency	IR Intensity
86.3	0.0
113.7	0.5
174.0	1.2
202.2	0.1
231.4	6.4
240.2	16.0
273.3	41.0
295.1	14.8
303.2	31.9
319.3	0.3
341.8	3.4
410.5	4.5
417.5	1.8
468.4	1.4
556.2	3.1
603.7	3.8
634.6	2.5
654.8	8.9
723.2	2.5
775.6	4.2
793.9	2.1
840.7	5.3
891.7	6.9
929.0	4.7
949.8	4.4
978.0	9.1
978.7	14.5
998.4	49.4
1017.4	4.8
1037.8	2.0
1060.9	2.7
1088.5	28.2
1101.7	0.3
1143.6	1.7
1181.4	23.4
1198.8	2.9
1227.9	0.6
1238.2	20.9
1252.4	24.3
1314.6	11.9
1317.7	2.0
1343.2	3.7
1350.2	6.0
1374.9	3.9
1400.6	16.6
1411.9	6.7
1420.1	5.9
1483.5	2.1
1486.0	6.6
1488.6	2.9
1499.0	5.6
1505.4	12.4
1505.9	5.2
1515.5	5.5
2434.1	73.9
3058.7	14.1
3062.9	18.7
3067.4	28.2
3074.1	8.8
3075.2	28.4
3103.8	2.0
3118.4	19.2
3127.8	44.1
3128.2	8.6
3130.5	15.0
3138.0	23.5
3142.1	9.3
3199.2	4.7
3877.0	28.0

Table S70: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
84.7	0.1
112.2	0.0
187.4	1.1
209.1	1.2
232.4	2.0
249.1	80.9
287.2	11.5
295.2	1.0
316.9	0.6
352.8	0.9
364.2	2.7
386.5	0.3
446.1	3.3
491.6	7.9
558.6	1.7
599.7	0.4
621.1	1.0
690.8	1.3
723.1	1.7
753.3	4.5
803.9	2.7
841.6	5.3
909.8	12.6
920.6	15.5
950.6	0.5
959.2	0.7
967.1	5.0
994.9	0.9
1016.4	7.6
1023.6	1.8
1065.5	1.9
1084.4	8.1
1109.5	26.4
1141.9	24.1
1175.5	31.4
1204.2	2.3
1210.4	24.1
1235.6	40.8
1257.8	6.3
1314.0	1.4
1320.4	16.6
1329.1	20.3
1359.1	1.4
1374.2	6.5
1394.1	21.3
1407.1	11.1
1412.0	8.1
1486.4	1.1
1492.8	1.6
1497.7	5.6
1506.0	14.8
1508.9	3.5
1511.9	1.4
1514.6	9.4
2424.7	76.6
3054.3	14.7
3058.3	33.4
3069.7	22.4
3073.8	14.9
3081.6	13.4
3112.6	5.7
3114.1	20.1
3122.7	27.2
3129.1	25.6
3131.2	26.0
3153.2	12.6
3157.8	20.1
3200.1	4.8
3871.6	30.3

Table S71: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
95.6	0.6
116.6	0.8
193.1	0.2
208.7	0.6
229.4	0.2
279.2	0.4
290.9	0.4
312.8	0.1
343.7	3.8
360.2	0.9
380.2	37.6
394.5	45.5
443.5	3.7
487.8	11.6
559.5	3.2
598.2	0.7
619.5	5.1
682.8	2.0
714.1	2.2
750.0	2.4
801.8	3.3
835.7	0.8
900.3	11.6
925.4	3.8
953.5	0.0
960.3	1.0
972.5	4.1
995.4	2.5
1017.2	34.5
1024.9	11.3
1064.7	2.7
1086.7	3.9
1105.8	11.5
1146.7	20.8
1168.8	9.3
1204.5	1.2
1228.0	34.4
1240.1	44.1
1248.5	14.8
1316.1	3.8
1325.1	12.7
1342.4	2.1
1361.5	2.8
1380.9	13.3
1384.6	48.2
1411.4	8.3
1419.1	34.6
1484.3	2.6
1489.8	4.5
1495.5	5.7
1504.9	14.5
1507.9	4.4
1510.4	0.8
1516.4	4.5
2443.7	65.5
3061.3	23.3
3068.9	10.2
3071.1	21.6
3072.2	20.2
3079.6	9.8
3110.3	5.9
3119.1	22.5
3131.8	23.7
3134.6	19.9
3145.3	24.4
3155.2	14.9
3161.0	14.1
3198.0	4.1
3835.8	20.1

Table S72: M06-2X/cc-pVTZ Frequencies and IR Intensities of trans-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol

Frequency	IR Intensity
78.1	0.2
109.4	0.5
204.2	1.7
214.6	0.3
221.3	1.2
241.6	22.0
256.4	66.5
282.9	1.2
294.0	3.7
314.7	0.6
363.8	5.1
401.0	3.7
416.0	3.5
475.2	3.9
558.7	2.6
610.1	3.5
614.2	0.8
686.3	6.7
719.5	4.9
757.1	2.4
818.4	16.2
828.8	1.7
905.8	6.7
914.4	13.3
951.0	2.7
964.3	0.6
965.5	18.9
1001.0	7.3
1012.3	4.5
1034.9	2.6
1064.2	1.1
1091.6	25.1
1101.0	25.2
1139.7	3.2
1176.2	23.6
1206.0	4.0
1207.3	5.7
1233.6	11.0
1254.7	35.5
1318.0	10.3
1319.9	6.2
1341.1	2.9
1360.1	1.0
1371.1	6.4
1391.8	8.7
1409.4	1.1
1413.2	35.4
1482.6	3.1
1485.4	4.0
1494.4	2.1
1497.3	4.8
1498.1	5.0
1502.0	8.7
1514.5	3.8
2436.9	69.3
3053.9	17.9
3068.7	30.6
3072.2	29.0
3073.1	16.1
3076.4	15.0
3107.4	11.6
3118.8	15.4
3123.0	21.4
3128.3	27.2
3128.6	26.9
3149.8	13.5
3173.1	8.0
3205.1	3.9
3867.6	28.5

Table S73: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-thiirane-1,2-dimethylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
123.1	0.2
210.2	33.6
216.2	11.1
223.4	43.9
242.8	9.6
277.1	0.8
328.6	2.1
332.7	0.9
357.9	0.4
383.4	1.0
434.8	6.4
497.8	11.8
573.5	3.2
619.7	1.0
629.6	2.4
679.1	14.4
774.1	0.8
836.3	6.2
914.7	2.7
943.1	4.7
950.0	2.2
985.3	0.9
990.7	8.0
1017.8	7.2
1059.5	1.8
1079.6	18.9
1102.8	34.9
1144.4	17.9
1188.8	37.1
1207.4	9.2
1238.6	2.3
1240.9	58.9
1268.9	2.0
1327.6	4.2
1333.6	23.0
1379.4	0.7
1399.1	32.6
1405.9	1.5
1415.3	6.5
1483.7	2.0
1489.3	12.2
1491.5	5.6
1498.6	11.0
1502.9	2.0
1514.4	1.1
3055.9	10.1
3061.3	25.3
3063.4	23.5
3094.7	22.6
3122.0	20.5
3124.7	17.7
3130.0	11.5
3151.0	9.6
3153.4	11.6
3156.9	8.5
3188.6	7.6
3874.2	34.3

Table S74: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-thiirane-1,2-dimethylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
122.6	2.6
217.3	0.7
228.2	0.2
233.2	0.2
272.7	0.8
323.8	0.7
326.5	0.6
352.5	1.2
378.9	3.0
415.1	64.3
436.6	28.8
502.1	19.2
572.7	6.7
613.0	0.4
630.4	5.4
673.9	11.0
767.5	1.0
832.6	3.1
914.4	0.2
946.6	3.1
959.1	1.4
986.6	8.5
992.4	3.8
1020.8	32.7
1058.6	9.4
1082.3	13.6
1103.8	6.6
1147.2	29.7
1169.7	8.4
1218.5	6.9
1243.2	38.0
1253.2	41.0
1273.4	1.1
1326.5	1.3
1346.6	7.9
1381.8	56.2
1398.9	15.3
1416.9	8.7
1421.5	20.6
1482.4	4.3
1485.3	3.6
1491.0	13.0
1496.9	8.6
1501.6	4.7
1515.9	0.4
3062.3	20.5
3063.2	12.5
3068.5	17.4
3101.8	11.9
3125.7	16.8
3130.0	9.3
3143.7	13.2
3147.2	15.4
3155.4	11.1
3158.0	11.1
3188.9	6.0
3830.5	23.5

Table S75: M06-2X/cc-pVTZ Frequencies and IR Intensities of trans-2,3-thiirane-1,2-dimethylcyclopentan-1-ol

Frequency	IR Intensity
118.8	1.0
206.9	0.5
222.9	1.9
238.5	10.2
250.4	5.5
260.8	79.9
299.6	4.5
330.3	1.5
340.8	2.6
392.1	4.7
416.0	2.5
468.6	2.3
581.7	8.5
620.4	0.8
632.0	4.0
679.9	27.4
788.7	7.0
832.3	1.1
907.7	4.6
930.9	6.0
955.9	21.0
982.5	5.5
995.8	0.3
1018.7	6.5
1061.6	10.5
1078.9	52.3
1096.9	9.1
1143.4	1.3
1189.8	34.7
1209.7	9.5
1231.9	2.0
1237.9	12.9
1264.8	22.3
1328.2	4.5
1346.1	6.3
1379.5	10.4
1401.6	8.1
1410.2	26.8
1415.4	3.2
1476.7	4.1
1486.3	8.3
1491.0	4.2
1494.6	5.8
1500.1	6.9
1503.0	3.0
3055.7	17.0
3070.5	18.2
3075.3	20.6
3094.2	23.7
3124.8	15.0
3130.2	13.6
3139.3	10.6
3146.5	6.2
3151.0	16.7
3157.3	6.9
3194.7	6.1
3872.8	34.3

Table S76: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol ((not H-bonded)

Frequency	IR Intensity
72.8	0.3
123.6	0.7
180.3	4.2
194.4	79.0
223.1	1.3
229.1	2.9
281.5	19.3
287.4	1.2
329.2	1.7
350.2	1.5
352.5	1.5
369.8	0.7
430.3	7.7
520.8	7.2
571.7	2.9
623.7	3.3
651.8	1.3
680.8	16.5
752.9	1.4
798.0	2.1
837.4	5.7
914.7	2.9
941.2	4.7
961.2	6.3
991.1	8.7
1015.8	9.8
1021.5	5.9
1043.1	16.0
1069.7	8.3
1079.0	10.7
1107.6	16.8
1143.7	16.0
1184.3	13.4
1198.9	17.8
1232.7	20.9
1234.9	36.6
1272.4	1.7
1312.0	3.8
1326.1	17.8
1331.5	0.3
1364.0	7.5
1384.2	0.3
1400.9	21.1
1412.9	2.2
1423.3	9.8
1478.8	2.9
1486.0	11.1
1497.2	8.7
1500.1	3.8
1502.2	4.8
1507.3	4.6
1517.3	9.5
3057.2	6.2
3061.0	25.4
3063.8	21.2
3067.9	24.7
3107.9	17.0
3115.0	6.9
3125.3	13.3
3131.6	21.2
3133.9	7.6
3143.3	30.2
3155.1	7.5
3157.2	16.8
3189.0	7.9
3881.8	33.7

Table S77: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol ((H-bonded)

Frequency	IR Intensity
130.9	1.7
158.0	0.3
213.2	0.3
235.4	0.2
241.9	1.1
259.8	0.2
281.4	0.1
324.1	1.5
342.8	0.5
357.9	0.4
415.4	8.1
419.1	67.0
457.8	24.6
496.7	13.0
576.8	8.2
614.2	0.4
636.1	3.0
675.3	13.8
757.8	0.4
798.1	3.9
836.7	2.2
915.1	0.8
935.3	17.0
962.9	5.4
988.7	1.7
1008.7	8.3
1037.1	9.7
1064.3	9.5
1074.2	32.9
1085.0	9.0
1114.3	12.5
1149.1	16.9
1173.7	10.9
1202.4	30.4
1230.2	18.6
1242.6	5.8
1258.9	6.4
1313.3	2.4
1327.3	0.3
1333.7	1.2
1374.1	44.0
1397.8	36.2
1401.5	11.0
1417.9	4.0
1420.7	5.5
1483.0	1.1
1487.8	14.3
1494.2	9.5
1499.9	4.8
1506.2	9.5
1508.2	5.2
1521.6	4.1
3062.4	6.0
3064.8	19.1
3076.8	15.4
3080.1	29.3
3098.5	14.4
3110.1	1.8
3125.1	14.2
3128.8	25.8
3134.0	16.4
3140.5	31.7
3144.0	11.8
3153.8	6.9
3188.9	5.7
3827.5	24.1

Table S78: M06-2X/cc-pVTZ Frequencies and IR Intensities of trans-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol

Frequency	IR Intensity
90.8	0.1
114.5	0.9
174.2	1.1
211.9	0.2
236.2	3.3
244.4	18.3
279.7	51.7
297.3	14.7
303.1	23.6
330.8	0.7
348.9	2.3
415.8	4.8
423.1	1.2
485.5	1.9
575.4	6.7
620.6	4.1
654.1	2.6
679.1	25.2
779.5	8.7
797.7	1.0
844.0	0.8
914.5	2.5
952.0	15.5
974.9	4.8
984.6	20.4
1002.5	30.9
1019.0	6.9
1036.3	2.2
1065.8	6.3
1082.5	25.6
1104.0	2.1
1147.1	1.2
1190.4	28.6
1202.9	7.8
1229.0	0.8
1237.1	19.0
1258.9	15.9
1317.6	5.7
1324.0	7.4
1344.4	3.8
1354.1	6.3
1388.4	9.1
1402.7	15.0
1414.4	5.1
1424.1	3.5
1478.0	3.7
1484.4	6.3
1488.5	3.2
1492.1	6.1
1503.1	7.4
1505.8	8.2
1515.2	6.1
3058.6	14.5
3067.7	11.5
3071.1	25.3
3075.0	21.5
3092.3	20.3
3106.0	1.2
3128.6	28.7
3129.4	11.5
3139.0	15.0
3140.4	18.7
3143.3	14.6
3156.6	6.3
3196.0	6.3
3878.2	31.3

Table S79: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-thiirane-1-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
86.7	0.3
112.0	0.2
187.3	1.8
210.0	2.6
227.1	76.8
235.0	12.1
281.1	4.9
295.1	0.8
335.4	1.4
356.8	1.1
369.2	1.5
387.8	1.0
445.7	5.0
505.7	11.2
568.4	2.6
625.0	3.8
636.1	1.3
715.1	14.1
755.7	1.7
809.6	4.0
840.4	10.8
913.2	7.5
945.4	2.6
951.1	0.9
968.5	5.7
997.0	4.9
1017.1	2.5
1030.7	4.5
1067.9	1.6
1084.9	9.7
1110.2	32.2
1145.4	18.7
1186.2	37.6
1207.4	7.8
1212.7	7.7
1238.7	48.5
1263.9	3.1
1314.0	4.8
1324.8	3.1
1332.7	23.5
1362.3	2.2
1384.4	2.2
1398.8	23.3
1406.5	5.6
1413.4	9.2
1482.9	3.1
1489.0	1.3
1495.9	8.9
1499.1	9.4
1505.9	4.0
1511.1	4.2
1515.3	9.0
3055.7	11.6
3058.1	26.7
3071.5	19.2
3076.9	13.4
3094.5	23.6
3122.1	19.0
3124.2	11.4
3124.8	18.2
3134.5	21.5
3151.6	10.5
3153.5	12.3
3160.0	18.4
3192.5	6.9
3874.3	34.2

Table S80: M06-2X/cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-thiirane-1-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
90.7	0.6
110.1	1.4
181.5	0.6
207.1	0.2
234.9	0.8
274.7	0.1
291.1	0.4
330.3	0.2
350.9	2.4
368.6	0.6
384.1	3.6
425.6	61.0
447.4	31.2
506.8	19.0
569.1	5.8
617.4	3.0
639.1	2.2
707.8	13.0
756.3	0.9
808.9	3.2
836.2	7.0
916.5	2.2
946.1	4.1
957.7	1.1
973.2	4.1
997.6	11.1
1022.2	16.3
1031.9	17.0
1069.0	7.9
1086.8	7.8
1108.1	8.8
1151.5	19.6
1170.3	10.5
1211.4	2.6
1233.7	23.5
1248.6	54.6
1253.5	5.2
1323.4	7.1
1323.7	5.8
1349.2	2.8
1364.0	1.7
1385.0	56.1
1400.0	6.0
1413.2	8.4
1421.1	29.0
1482.7	3.4
1485.7	6.1
1493.3	4.3
1499.5	12.4
1505.3	4.7
1511.2	3.6
1516.1	4.0
3059.1	20.3
3069.0	6.7
3071.6	18.9
3075.7	17.6
3102.8	12.6
3121.8	2.9
3126.7	18.5
3135.0	21.6
3145.4	15.3
3148.0	16.4
3154.3	17.6
3164.7	13.7
3193.1	5.5
3828.4	23.8

Table S81: M06-2X/cc-pVTZ Frequencies and IR Intensities of trans-2-ethyl-2,3-thiirane-1-methylcyclopentan-1-ol

Frequency	IR Intensity
61.8	0.1
112.0	0.8
191.9	0.7
215.7	0.3
228.6	2.5
249.0	2.7
269.5	64.1
274.5	24.4
299.8	4.2
331.4	1.5
371.2	4.0
407.5	6.1
415.3	1.7
483.0	4.5
576.3	7.3
622.9	2.5
635.5	1.6
712.4	23.3
764.3	2.6
816.3	14.1
841.1	5.2
903.7	9.9
934.7	3.4
962.8	16.1
970.2	4.9
997.7	9.9
1014.2	1.8
1040.2	3.9
1067.2	0.3
1096.4	13.3
1099.6	40.3
1143.9	1.8
1186.4	30.9
1206.0	4.3
1214.6	2.1
1234.1	12.8
1259.7	21.7
1316.2	11.6
1326.4	4.8
1344.9	4.0
1361.9	1.0
1387.6	5.0
1398.9	2.1
1409.5	2.1
1412.6	36.0
1476.5	3.1
1484.8	5.1
1490.8	5.4
1495.5	3.4
1499.4	2.1
1501.5	8.9
1516.4	5.1
3055.4	16.6
3069.3	24.4
3071.3	20.8
3074.3	19.3
3094.0	23.2
3116.9	9.7
3124.5	11.9
3129.1	19.3
3130.4	27.8
3146.2	9.0
3153.9	14.3
3177.5	7.0
3197.2	5.4
3869.3	33.3

Table S82: M06-2X optimized geometry of cis-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.255493	0.784830	−0.022740
C	−1.554546	0.188680	−0.347625
C	−1.430016	−1.314834	−0.423343
C	−0.120823	−1.588670	0.333592
C	0.758241	−0.345139	0.097911
C	1.566518	−0.468303	−1.188670
H	2.240613	−1.324255	−1.121017
H	0.912941	−0.621023	−2.049095
H	2.164080	0.426653	−1.354247
O	1.614951	−0.055560	1.190538
H	2.254187	−0.766851	1.283788
H	−0.317766	−1.658299	1.400779
H	0.373347	−2.503721	0.007701
H	−2.284246	−1.825873	0.019666
H	−1.362849	−1.619889	−1.469479
O	−1.284805	0.689921	0.956300
H	−2.312540	0.726117	−0.904406
C	0.184969	2.169874	−0.380957
H	0.626311	2.199598	−1.376412
H	−0.670008	2.842405	−0.356307
H	0.927404	2.517708	0.337614

Table S83: M06-2X optimized geometry of cis-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.018512	−0.004782	0.019634
C	1.527000	−0.031630	0.023641
C	1.982660	1.434289	0.012010
C	0.854397	2.140833	−0.699030
C	−0.352579	1.316229	−0.667411
C	−1.759093	1.823338	−0.716416
H	−2.417694	1.057311	−1.127601
H	−2.115196	2.081632	0.280146
H	−1.810103	2.707766	−1.348235
O	0.412243	1.452660	−1.869412
H	0.811641	3.221212	−0.762621
H	2.068607	1.837132	1.023115
H	2.942682	1.572738	−0.484315
H	1.913677	−0.592724	0.872138
H	1.863813	−0.527941	−0.884775
O	−0.575786	−1.101447	−0.684308
H	−0.261801	−1.054317	−1.593566
C	−0.593546	−0.053831	1.422227
H	−0.302927	−0.988134	1.900248
H	−0.217954	0.778929	2.018825
H	−1.681048	−0.006217	1.392921

Table S84: M06-2X optimized geometry of trans-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
C	0.726363	−0.410665	0.005332
C	−0.226451	−1.588396	0.276265
C	−1.571997	−1.183458	−0.345589
C	−1.565459	0.318867	−0.218861
C	−0.198135	0.800920	−0.018248
O	−1.122699	0.766564	1.063869
H	−2.327766	0.933381	−0.681078
H	−1.616498	−1.446942	−1.402938
H	−2.421082	−1.643657	0.158516
H	0.176260	−2.510163	−0.143221
H	−0.336807	−1.724767	1.350146
C	0.324877	2.142733	−0.420160
H	−0.492683	2.858486	−0.480742
H	1.042718	2.505511	0.317063
H	0.822795	2.076562	−1.385462
C	1.843321	−0.293307	1.025070
H	2.415978	−1.222205	1.073949
H	2.521261	0.515660	0.753916
H	1.429459	−0.095624	2.013674
O	1.249021	−0.480778	−1.321148
H	1.868244	−1.214063	−1.367232

Table S85: M06-2X optimized geometry of cis-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.920003	0.588809	−0.105052
C	−1.713443	−0.548525	−0.579605
C	−0.908341	−1.820775	−0.466967
C	0.195511	−1.439751	0.531935
C	0.449859	0.065441	0.312889
C	1.466934	0.330035	−0.804094
C	2.888663	−0.103876	−0.467425
H	2.957990	−1.171669	−0.261224
H	3.559648	0.111783	−1.297538
H	3.268139	0.438465	0.399289
H	1.125543	−0.173476	−1.712837
H	1.469665	1.400619	−1.012445
O	0.830464	0.742225	1.500375
H	1.591323	0.299548	1.884376
H	−0.169639	−1.567724	1.548443
H	1.095383	−2.039691	0.410150
H	−1.507459	−2.663932	−0.124268
H	−0.496604	−2.077877	−1.444859
O	−1.967528	0.040856	0.689637
H	−2.503446	−0.436268	−1.312230
C	−1.104142	2.013829	−0.527731
H	−0.574357	2.227873	−1.454697
H	−2.163646	2.211043	−0.677699
H	−0.728984	2.680934	0.248807

Table S86: M06-2X optimized geometry of cis-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	0.425930	0.099496	0.664434
C	−0.652805	0.604099	−0.289708
C	−1.372871	−0.541382	−0.844691
C	−0.758014	−1.830641	−0.361927
C	0.080680	−1.399546	0.852546
H	0.979063	−2.001872	0.980157
H	−0.507985	−1.496996	1.762632
H	−0.138755	−2.245736	−1.158211
H	−1.512836	−2.573476	−0.104717
O	−1.942434	0.232085	0.210905
H	−1.903213	−0.485165	−1.787710
C	−0.554299	1.961222	−0.910969
H	−1.469700	2.187000	−1.454237
H	−0.409315	2.714575	−0.135572
H	0.287987	2.015054	−1.600490
O	0.367331	0.815278	1.887980
H	−0.538284	0.759625	2.211775
C	1.829721	0.330861	0.121493
C	2.117593	−0.381171	−1.194635
H	1.398023	−0.107083	−1.968211
H	3.110651	−0.123897	−1.559258
H	2.082547	−1.464510	−1.077348
H	1.975055	1.407154	0.012979
H	2.529728	−0.000923	0.890293

Table S87: M06-2X optimized geometry of trans-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.467271	−0.009888	0.212898
C	0.887398	0.636627	−0.054880
C	1.903153	−0.416460	−0.033628
C	1.261073	−1.748027	0.258162
C	−0.218895	−1.502530	−0.075612
H	−0.891145	−2.130237	0.508838
H	−0.402922	−1.702754	−1.129855
H	1.395961	−1.979203	1.315445
H	1.691280	−2.559864	−0.327333
O	1.461502	0.155584	−1.266165
H	2.935120	−0.212415	0.223130
C	1.117377	2.076531	0.277155
H	2.166482	2.328569	0.134582
H	0.520876	2.716332	−0.374668
H	0.833484	2.271978	1.309389
C	−1.583017	0.601249	−0.625246
C	−2.928144	−0.094378	−0.449805
H	−2.873915	−1.144144	−0.739000
H	−3.275562	−0.044508	0.584259
H	−3.693140	0.379542	−1.062751
H	−1.674480	1.654590	−0.352446
H	−1.274462	0.559559	−1.671959
O	−0.687571	0.203240	1.606953
H	−1.504788	−0.233887	1.859301

Table S88: M06-2X optimized geometry of cis-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.398510	−0.289825	0.375019
C	0.078513	−1.563641	−0.174546
C	1.415778	−1.369109	−0.849866
C	1.915260	−0.048195	−0.244164
C	0.646854	0.773380	0.060196
C	0.222785	1.611278	−1.139727
H	1.002740	2.339483	−1.371099
H	0.070303	0.988449	−2.022532
H	−0.697884	2.152350	−0.924556
O	0.784629	1.600768	1.204489
H	1.436804	2.282027	1.020500
H	2.419210	−0.241281	0.699848
H	2.598078	0.487993	−0.902957
H	2.099083	−2.197851	−0.666753
H	1.267766	−1.288831	−1.928600
O	0.132658	−1.306787	1.222071
H	−0.599118	−2.353391	−0.475507
C	−1.843300	0.083049	0.592495
C	−2.710748	−0.009327	−0.661081
H	−2.717950	−1.026955	−1.051724
H	−3.739775	0.269351	−0.436867
H	−2.353442	0.646924	−1.453135
H	−2.234666	−0.586918	1.357520
H	−1.878477	1.091676	1.009336

Table S89: M06-2X optimized geometry of cis-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−1.846771	−0.013084	0.594264
C	−0.391258	−0.310166	0.351055
C	0.135393	−1.570901	−0.171976
C	1.429847	−1.325501	−0.908181
C	1.895318	0.028790	−0.355578
C	0.615970	0.798198	0.050099
C	0.137015	1.723543	−1.051327
H	−0.788374	2.220329	−0.762262
H	0.894052	2.486144	−1.229200
H	−0.029076	1.169320	−1.976064
O	0.817829	1.612895	1.192674
H	1.064212	1.033859	1.921965
H	2.499031	−0.126124	0.536648
H	2.492388	0.596828	−1.066378
H	2.160043	−2.118337	−0.748713
H	1.221192	−1.273773	−1.978630
O	0.218267	−1.274156	1.220882
H	−0.509223	−2.404992	−0.421767
H	−2.211780	−0.753793	1.305915
H	−1.924704	0.961669	1.081390
C	−2.705631	−0.050779	−0.668019
H	−2.383399	0.685474	−1.402034
H	−2.656292	−1.033407	−1.137674
H	−3.748232	0.153267	−0.427644

Table S90: M06-2X optimized geometry of trans-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
C	0.559364	0.805161	−0.011993
C	1.886259	0.085727	−0.321334
C	1.498462	−1.317803	−0.810662
C	0.212278	−1.588159	−0.071840
C	−0.382192	−0.329158	0.382047
C	−1.857233	−0.113777	0.587548
H	−2.010168	0.804892	1.158805
C	−2.666547	−0.067448	−0.706132
H	−2.522529	−0.984108	−1.279064
H	−3.729170	0.027366	−0.485146
H	−2.362841	0.768484	−1.329995
H	−2.205682	−0.934789	1.215591
O	0.269169	−1.205024	1.301802
H	−0.391042	−2.463636	−0.279181
H	1.296889	−1.324632	−1.882567
H	2.267734	−2.060367	−0.601594
H	2.460601	0.648637	−1.056960
H	2.479384	0.012924	0.587833
C	0.697579	1.864147	1.066216
H	0.991944	1.403589	2.008770
H	1.462782	2.592308	0.787515
H	−0.244890	2.392789	1.205458
O	0.000044	1.361642	−1.201231
H	0.550053	2.099490	−1.478365

Table S91: M06-2X optimized geometry of cis-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	0.972450	0.008630	0.224321
C	−0.329106	0.609555	−0.291182
C	−1.106261	−0.478317	−0.921030
C	−0.344928	−1.780816	−0.804913
C	0.658116	−1.496903	0.324716
C	−0.363318	2.042186	−0.735785
N	−1.493204	0.043295	0.396142
C	2.108684	0.268478	−0.759283
O	1.273542	0.598460	1.479792
H	3.012436	−0.243408	−0.423375
H	1.858753	−0.105516	−1.753595
H	2.324391	1.333544	−0.827163
H	2.079281	0.203798	1.823584
H	0.188396	−1.672875	1.289254
H	1.559526	−2.105867	0.253439
H	−0.994449	−2.625844	−0.577639
H	0.166291	−1.991706	−1.746133
H	−1.750487	−0.284296	−1.768474
H	0.327682	2.223522	−1.558310
H	−1.364250	2.310254	−1.075626
H	−0.091059	2.698732	0.091700
H	−2.274401	0.681869	0.299125

Table S92: M06-2X optimized geometry of cis-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	0.300664	−0.755435	−0.053001
C	−0.788877	0.302634	0.119994
C	0.000260	1.628316	0.235479
C	1.319667	1.413597	−0.519019
C	1.563102	−0.071722	−0.382757
C	−0.060563	−2.141894	−0.494328
C	−1.745618	0.316398	−1.056702
N	1.323999	−0.565515	0.985575
O	−1.568838	0.042166	1.274198
H	−0.790116	−2.578731	0.189704
H	−0.492882	−2.138409	−1.494398
H	0.823343	−2.780470	−0.512606
H	2.324021	−0.564134	−0.973884
H	1.216459	1.661360	−1.577201
H	2.133751	2.013171	−0.112270
H	−0.576578	2.469718	−0.144336
H	0.205249	1.811247	1.288336
H	−0.952548	−0.041409	2.010710
H	−2.473211	1.115600	−0.923220
H	−1.202464	0.486854	−1.987696
H	−2.283007	−0.628100	−1.127910
H	1.826616	−1.435187	1.123291

Table S93: M06-2X optimized geometry of trans-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
C	0.300664	−0.755435	−0.053001
C	−0.788877	0.302634	0.119994
C	0.000260	1.628316	0.235479
C	1.319667	1.413597	−0.519019
C	1.563102	−0.071722	−0.382757
C	−0.060563	−2.141894	−0.494328
C	−1.745618	0.316398	−1.056702
N	1.323999	−0.565515	0.985575
O	−1.568838	0.042166	1.274198
H	−0.790116	−2.578731	0.189704
H	−0.492882	−2.138409	−1.494398
H	0.823343	−2.780470	−0.512606
H	2.324021	−0.564134	−0.973884
H	1.216459	1.661360	−1.577201
H	2.133751	2.013171	−0.112270
H	−0.576578	2.469718	−0.144336
H	0.205249	1.811247	1.288336
H	−0.952548	−0.041409	2.010710
H	−2.473211	1.115600	−0.923220
H	−1.202464	0.486854	−1.987696
H	−2.283007	−0.628100	−1.127910
H	1.826616	−1.435187	1.123291

Table S94: M06-2X optimized geometry of cis-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.958535	0.570540	−0.083280
C	−1.782226	−0.570033	−0.551000
C	−0.962012	−1.839976	−0.498849
C	0.190220	−1.498013	0.455663
C	0.411305	0.026108	0.318771
C	1.455039	0.357987	−0.753059
C	2.878815	−0.057087	−0.398383
H	2.963180	−1.123684	−0.190518
H	3.556103	0.168516	−1.220675
H	3.245992	0.490969	0.470569
H	1.146455	−0.119056	−1.687570
H	1.439150	1.434593	−0.923081
O	0.760393	0.630154	1.559615
H	1.606972	0.281820	1.850996
H	−0.079836	−1.717176	1.488406
H	1.089816	−2.070021	0.236984
H	−1.537710	−2.703898	−0.164201
H	−0.586146	−2.066108	−1.498494
H	−2.535535	−0.449975	−1.318816
C	−1.083275	1.975734	−0.600593
H	−0.603411	2.096643	−1.571451
H	−2.137766	2.223673	−0.700779
H	−0.630118	2.677398	0.101434
N	−2.080519	0.088962	0.714796
H	−1.771060	−0.451086	1.514906

Table S95: M06-2X optimized geometry of cis-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
N	−1.980638	0.237658	0.215452
C	−0.660194	0.607651	−0.319759
C	0.413858	0.111857	0.649192
C	0.069044	−1.386288	0.850951
C	−0.750118	−1.834808	−0.370286
C	−1.378700	−0.555460	−0.869702
O	0.345305	0.836811	1.866179
C	1.825234	0.331295	0.119761
C	2.131674	−0.408177	−1.176885
C	−0.495521	1.924543	−1.017202
H	0.966482	−1.985291	1.001326
H	−0.535366	−1.469990	1.751640
H	−0.111913	−2.247583	−1.152629
H	−1.495105	−2.587461	−0.112395
H	−1.841704	−0.512678	−1.847044
H	−1.373251	2.148887	−1.624484
H	−0.366581	2.723829	−0.285294
H	0.375475	1.923254	−1.672221
H	−0.572749	0.793569	2.157988
H	1.414061	−0.162967	−1.961744
H	3.124767	−0.148614	−1.540358
H	2.107366	−1.488460	−1.033024
H	1.976329	1.404825	−0.006956
H	2.514236	0.012991	0.904105
H	−2.682989	0.860027	−0.168576

Table S96: M06-2X optimized geometry of trans-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.444768	−0.014081	0.174599
C	0.908805	0.633835	−0.105878
C	1.937321	−0.430257	−0.045300
C	1.273636	−1.750203	0.277537
C	−0.206084	−1.517622	−0.065015
H	−0.875718	−2.119149	0.548792
H	−0.418598	−1.776822	−1.103644
H	1.391859	−1.953967	1.342034
H	1.702043	−2.588214	−0.273553
H	2.941249	−0.232528	0.306067
C	1.130949	2.058614	0.309566
H	2.168547	2.331448	0.126886
H	0.500660	2.732988	−0.272621
H	0.900370	2.191610	1.364535
C	−1.569754	0.575484	−0.670795
C	−2.918791	−0.102446	−0.458524
H	−2.875682	−1.164072	−0.703943
H	−3.259006	−0.006454	0.574399
H	−3.684433	0.351789	−1.085433
H	−1.648558	1.637812	−0.433033
H	−1.282835	0.503115	−1.722883
O	−0.675959	0.223935	1.563410
H	−1.499367	−0.201559	1.815717
N	1.592152	0.197751	−1.319940
H	1.020443	−0.411712	−1.894061

Table S97: M06-2X optimized geometry of cis-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.391981	−0.324865	0.423473
C	0.081197	−1.620633	−0.124612
C	1.382888	−1.411789	−0.869418
C	1.908666	−0.077489	−0.323570
C	0.655727	0.732083	0.079528
C	0.202892	1.632492	−1.061446
H	0.981508	2.366714	−1.280345
H	0.024633	1.052240	−1.967754
H	−0.709000	2.165676	−0.796956
O	0.874862	1.510596	1.251658
H	1.456587	2.244544	1.036268
H	2.523768	−0.231467	0.562497
H	2.519550	0.460246	−1.048067
H	2.089383	−2.230054	−0.724931
H	1.176778	−1.342753	−1.939214
H	−0.609010	−2.383532	−0.460630
C	−1.845437	0.067128	0.567380
C	−2.660394	−0.013725	−0.721512
H	−2.633204	−1.024493	−1.129585
H	−3.703123	0.239743	−0.532023
H	−2.290120	0.663013	−1.489704
H	−2.281619	−0.600043	1.309639
H	−1.893782	1.074553	0.988237
N	0.081969	−1.382296	1.312456
H	1.008962	−1.186325	1.673073

Table S98: M06-2X optimized geometry of cis-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
N	0.249763	−1.323545	1.234733
C	−0.406334	−0.337407	0.357716
C	0.611646	0.761584	0.039410
C	1.863081	−0.019219	−0.431378
C	1.357489	−1.356670	−0.989271
C	0.092185	−1.606862	−0.201621
C	−1.865949	−0.008759	0.556900
C	−2.696552	−0.010946	−0.724945
C	0.124310	1.726033	−1.024385
O	0.872814	1.542901	1.192842
H	−0.784024	2.234368	−0.702776
H	0.893050	2.477774	−1.198481
H	−0.071459	1.200898	−1.960096
H	1.108765	0.924979	1.894389
H	2.497230	−0.198468	0.434214
H	2.439555	0.553426	−1.155820
H	2.089223	−2.156601	−0.877808
H	1.106251	−1.275940	−2.048707
H	−0.591479	−2.394520	−0.490748
H	−2.294717	−0.736787	1.249590
H	−1.934802	0.961741	1.054488
H	−2.347297	0.733991	−1.436402
H	−2.648240	−0.985078	−1.212196
H	−3.742121	0.202436	−0.504599
H	−0.457350	−1.829327	1.755702

Table S99: M06-2X optimized geometry of trans-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
N	0.233235	−1.183307	1.368451
C	0.051907	−1.592464	−0.033333
C	1.313700	−1.437006	−0.848715
C	1.844360	−0.064364	−0.407657
C	0.599247	0.771347	−0.053920
C	−0.414225	−0.266593	0.420080
C	0.883316	1.847063	0.978171
O	0.034760	1.346169	−1.234457
C	−1.871467	0.091803	0.584714
C	−2.675850	0.093230	−0.713188
H	−1.945871	1.068717	1.068593
H	−2.617653	−0.881243	−1.199124
H	−3.725395	0.305988	−0.510163
H	−2.294227	0.837256	−1.406016
H	−2.317819	−0.626019	1.278039
H	−0.655562	−2.381934	−0.250535
H	1.055184	−1.434775	−1.908258
H	2.034007	−2.234958	−0.670333
H	2.430230	0.434008	−1.180401
H	2.468062	−0.173054	0.476663
H	1.201719	1.389295	1.913843
H	1.680227	2.508232	0.629656
H	−0.006718	2.450249	1.156877
H	0.646255	2.008604	−1.567141
H	−0.478550	−1.619240	1.943267

Table S100: M06-2X optimized geometry of cis-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	0.980799	−0.012171	0.250281
C	−0.342497	0.592476	−0.228646
C	−1.116033	−0.506080	−0.882842
C	−0.291959	−1.783654	−0.835632
C	0.702068	−1.526441	0.302187
C	−0.321612	1.995483	−0.776954
P	−1.814510	0.014620	0.772125
C	2.104558	0.294218	−0.736960
O	1.302253	0.531572	1.522242
H	3.015319	−0.223877	−0.429279
H	1.848092	−0.043781	−1.741998
H	2.309454	1.362721	−0.767936
H	2.185779	0.244809	1.768490
H	0.247278	−1.754701	1.266634
H	1.615298	−2.114611	0.213264
H	−0.894426	−2.676049	−0.671805
H	0.235572	−1.909166	−1.784264
H	−1.708381	−0.293968	−1.762440
H	0.303164	2.057337	−1.670589
H	−1.324134	2.320108	−1.049596
H	0.072090	2.690013	−0.034291
H	−2.690089	0.977921	0.217574

Table S101: M06-2X optimized geometry of cis-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	0.970213	−0.000542	0.241997
C	−0.341213	0.600643	−0.293113
C	−1.106732	−0.500377	−0.936697
C	−0.288661	−1.780724	−0.857954
C	0.687456	−1.515967	0.292376
C	−0.307873	1.996827	−0.856023
P	−1.838880	0.038797	0.699716
C	2.129198	0.300835	−0.696988
O	1.351383	0.531907	1.497012
H	3.024120	−0.198784	−0.328703
H	1.914472	−0.055200	−1.705248
H	2.324932	1.370625	−0.733410
H	0.592661	0.475395	2.087749
H	0.218636	−1.754055	1.248980
H	1.604506	−2.098054	0.224826
H	−0.898394	−2.668809	−0.698826
H	0.253762	−1.913845	−1.796838
H	−1.696719	−0.302265	−1.821368
H	0.335616	2.041310	−1.736940
H	−1.303166	2.323515	−1.152092
H	0.078464	2.699706	−0.117216
H	−2.699758	1.010236	0.140930

Table S102: M06-2X optimized geometry of trans-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.300143	0.610637	−0.274278
C	1.029986	−0.008206	0.168457
C	0.703625	−1.497843	0.354353
C	−0.347644	−1.796843	−0.721025
C	−1.136422	−0.501896	−0.814353
C	1.655217	0.641901	1.388486
O	1.891122	0.148323	−0.965505
P	−1.741951	0.154827	0.830193
C	−0.251039	1.967745	−0.925639
H	−1.767271	−0.328134	−1.675076
H	0.140533	−1.980752	−1.679349
H	−0.964121	−2.660911	−0.478227
H	1.601710	−2.108648	0.261003
H	0.292558	−1.665307	1.351310
H	−1.234849	2.246761	−1.300416
H	0.067686	2.734785	−0.218761
H	0.451934	1.956011	−1.758065
H	2.594922	0.146254	1.642962
H	1.866529	1.692241	1.189146
H	0.988408	0.571391	2.246893
H	2.749120	−0.225013	−0.746017
H	−2.605618	1.119228	0.260670

Table S103: M06-2X optimized geometry of cis-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	0.406452	−1.473601	0.338795
C	0.637332	0.050294	0.296603
C	−0.680974	0.599965	−0.265632
C	−1.371316	−0.528284	−0.960747
C	−0.502008	−1.770879	−0.858755
C	1.801195	0.427588	−0.633229
C	3.166977	−0.082735	−0.186172
O	0.848444	0.607818	1.585545
C	−0.698697	2.002662	−0.817680
P	−2.185452	−0.037113	0.649365
H	3.212756	−1.169972	−0.140518
H	3.937567	0.246096	−0.882129
H	3.441197	0.312388	0.793456
H	1.578433	0.059640	−1.638423
H	1.840821	1.515120	−0.693014
H	1.660028	0.247516	1.951880
H	−0.106486	−1.708317	1.272143
H	1.332428	−2.044800	0.320090
H	−1.076356	−2.687306	−0.729687
H	0.089439	−1.875811	−1.771615
H	−1.917287	−0.340372	−1.875233
H	−0.048888	2.091552	−1.690484
H	−1.704554	2.282447	−1.125183
H	−0.362259	2.715235	−0.063984
H	−3.066020	0.890274	0.044212

Table S104: M06-2X optimized geometry of cis-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.365735	1.473612	0.738590
C	−0.569293	−0.057603	0.674323
C	0.480619	−0.527860	−0.348108
C	0.961208	0.660333	−1.101486
C	0.215514	1.895153	−0.618324
O	−0.405743	−0.678596	1.938827
C	−1.991202	−0.439178	0.257356
C	−2.486869	0.185989	−1.040205
C	0.306273	−1.881389	−0.985646
P	2.219276	0.028467	0.128443
H	−1.291354	1.991314	0.987228
H	0.346601	1.688198	1.536734
H	−0.577093	2.131737	−1.328455
H	0.859663	2.769867	−0.538922
H	1.213945	0.571453	−2.149732
H	1.134918	−2.107338	−1.654619
H	0.259724	−2.659777	−0.223368
H	−0.616383	−1.923569	−1.567902
H	0.523365	−0.614946	2.184709
H	−1.800533	0.006075	−1.869426
H	−3.455206	−0.230535	−1.313671
H	−2.612497	1.263864	−0.940404
H	−2.041596	−1.527116	0.201627
H	−2.642270	−0.144347	1.082235
H	2.859034	−0.856811	−0.768171

Table S105: M06-2X optimized geometry of trans-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
P	1.642051	0.078177	−1.763408
C	0.886774	0.630761	−0.141033
C	−0.473506	−0.011572	0.154774
C	−0.225620	−1.516076	−0.046920
C	1.224086	−1.730629	0.405710
C	1.917096	−0.437962	0.013480
C	−1.616075	0.554396	−0.680958
C	−2.969916	−0.077665	−0.378028
O	−0.692340	0.247664	1.545986
C	1.113391	2.035699	0.353299
H	−0.938333	−2.116627	0.517964
H	−0.343304	−1.772254	−1.101779
H	1.263132	−1.834509	1.491220
H	1.675916	−2.615768	−0.039426
H	2.875291	−0.197781	0.453120
H	2.150853	2.330016	0.200190
H	0.481545	2.750204	−0.175369
H	0.884115	2.097042	1.416799
H	−2.955381	−1.153911	−0.553990
H	−3.275299	0.096277	0.655436
H	−3.745765	0.349221	−1.011709
H	−1.664241	1.630771	−0.503282
H	−1.369308	0.411074	−1.734283
H	−1.487814	−0.216771	1.819084
H	2.637663	1.082772	−1.751906

Table S106: M06-2X optimized geometry of cis-2-ethyl-2,3-phosphirane-methylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.319077	1.019309	−0.313250
C	0.328837	−0.367173	−0.200332
C	−0.288421	−1.042676	0.983841
C	−1.275853	−0.086583	1.634995
C	−1.616424	0.895775	0.509225
C	1.798558	−0.507705	−0.563202
C	2.765088	−0.308998	0.604618
P	−0.871730	−1.737393	−0.647896
C	0.569516	2.114903	0.271031
O	−0.559125	1.293407	−1.686474
H	1.518539	2.175994	−0.259006
H	0.060924	3.077262	0.177625
H	0.763990	1.942988	1.329683
H	−0.848511	2.205394	−1.775511
H	−2.392219	0.483631	−0.136616
H	−1.961891	1.862494	0.875283
H	−2.156649	−0.588424	2.033366
H	−0.785832	0.432390	2.462543
H	0.309503	−1.685836	1.614133
H	1.980040	−1.493293	−0.988779
H	2.012770	0.204429	−1.362995
H	2.669304	0.674441	1.059935
H	2.589735	−1.052786	1.382119
H	3.795359	−0.421699	0.267026
H	0.134676	−2.730763	−0.701253

Table S107: M06-2X optimized geometry of cis-2-ethyl-2,3-phosphirane-methylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.366889	1.000142	−0.268742
C	0.302598	−0.383485	−0.144692
C	−0.290191	−1.058134	1.042858
C	−1.269076	−0.104967	1.712195
C	−1.639229	0.874830	0.594892
C	1.763402	−0.523471	−0.537439
C	2.748124	−0.282747	0.607031
P	−0.910576	−1.766211	−0.571919
C	0.519428	2.118190	0.261331
O	−0.641153	1.352820	−1.612489
H	1.456473	2.170496	−0.290117
H	−0.005737	3.063790	0.132000
H	0.734229	1.977211	1.320349
H	−1.088331	0.608999	−2.030455
H	−2.443666	0.464826	−0.018139
H	−1.970677	1.844345	0.961922
H	−2.135872	−0.611005	2.134686
H	−0.757907	0.415938	2.525354
H	0.314044	−1.710210	1.658301
H	1.945910	−1.519219	−0.938790
H	1.955185	0.171067	−1.358375
H	2.648608	0.712577	1.034079
H	2.593862	−1.006027	1.408033
H	3.773044	−0.394954	0.253820
H	0.094425	−2.754288	−0.669719

Table S108: M06-2X optimized geometry of trans-2-ethyl-2,3-phosphirane-methylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.369613	−0.292152	0.247267
C	0.461477	0.998149	0.195602
C	1.683650	0.626364	−0.659322
C	1.154772	−0.397879	−1.668459
C	0.097500	−1.153207	−0.882246
C	0.825095	1.570601	1.553920
O	−0.353642	1.935002	−0.518739
P	0.652170	−1.767410	0.792516
C	−1.836069	−0.169219	0.629659
C	−2.765092	0.071404	−0.559193
H	−1.933857	0.653980	1.339827
H	−2.744645	−0.775276	−1.245871
H	−3.793177	0.193344	−0.217653
H	−2.470476	0.963005	−1.106264
H	−2.158453	−1.067272	1.155763
H	−0.611715	−1.769278	−1.416555
H	0.671671	0.113553	−2.503052
H	1.938610	−1.040697	−2.066183
H	2.113400	1.511976	−1.127265
H	2.453655	0.178633	−0.028817
H	1.421536	0.861121	2.125460
H	1.407052	2.487489	1.432909
H	−0.075299	1.810781	2.118914
H	0.106393	2.778833	−0.538775
H	−0.471776	−2.603858	0.983731

Table S109: M06-2X optimized geometry of cis-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.264769	0.792344	0.051282
C	−1.573866	0.195527	−0.304475
C	−1.415122	−1.307067	−0.447696
C	−0.117036	−1.613830	0.309694
C	0.749479	−0.350913	0.142924
C	1.569732	−0.425242	−1.143833
H	2.227444	−1.295763	−1.107748
H	0.924486	−0.527970	−2.017912
H	2.183552	0.465680	−1.261609
O	1.606038	−0.109521	1.245402
H	2.289896	−0.784318	1.262452
H	−0.317521	−1.751532	1.369342
H	0.387623	−2.502901	−0.067693
H	−2.270350	−1.860387	−0.063906
H	−1.312809	−1.546418	−1.509277
S	−1.488644	0.818386	1.399279
H	−2.252572	0.729639	−0.956327
C	0.189843	2.128738	−0.469831
H	0.525429	2.048278	−1.504954
H	−0.626592	2.845846	−0.424646
H	1.016230	2.504795	0.133122

Table S110: M06-2X optimized geometry of cis-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.010101	−0.027189	−0.018760
C	1.532801	−0.040359	0.038916
C	1.957035	1.431479	0.045301
C	0.858124	2.135151	−0.726547
C	−0.351105	1.289220	−0.739667
C	−1.743867	1.845534	−0.636744
H	−2.471154	1.103686	−0.966849
H	−1.972789	2.114254	0.395573
H	−1.844365	2.732306	−1.258557
S	0.473835	1.437439	−2.368394
H	0.766544	3.212066	−0.674097
H	1.965010	1.829959	1.063070
H	2.945054	1.593386	−0.381664
H	1.891199	−0.588250	0.908134
H	1.913973	−0.538510	−0.850319
O	−0.546164	−1.156295	−0.676095
H	−0.222153	−1.144187	−1.583875
C	−0.609170	−0.033889	1.379673
H	−0.301001	−0.943344	1.892911
H	−0.264948	0.828280	1.952846
H	−1.696277	−0.017696	1.332357

Table S111: M06-2X optimized geometry of trans-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
C	0.723434	−0.397437	0.058157
C	−0.217776	−1.593633	0.272143
C	−1.541222	−1.174146	−0.379920
C	−1.576358	0.328869	−0.194862
C	−0.205046	0.823197	0.061451
S	−1.306939	0.918963	1.508815
H	−2.266473	0.928696	−0.772672
H	−1.521586	−1.381581	−1.451542
H	−2.405420	−1.676721	0.050192
H	0.204314	−2.494997	−0.172330
H	−0.354289	−1.773293	1.336185
C	0.314593	2.118089	−0.498511
H	−0.476794	2.864897	−0.506500
H	1.135182	2.500276	0.108870
H	0.680184	1.961919	−1.512322
C	1.858880	−0.321683	1.059715
H	2.463670	−1.230057	1.014354
H	2.502702	0.529310	0.838788
H	1.467096	−0.221684	2.071013
O	1.237539	−0.424139	−1.277892
H	1.825028	−1.180186	−1.360013

Table S112: M06-2X optimized geometry of cis-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.943863	0.593268	−0.036660
C	−1.738503	−0.551637	−0.540220
C	−0.891442	−1.808212	−0.480185
C	0.214714	−1.458408	0.522735
C	0.437948	0.058740	0.362110
C	1.446518	0.373231	−0.754939
C	2.868453	−0.097821	−0.470634
H	2.934295	−1.177866	−0.346056
H	3.527623	0.175797	−1.293268
H	3.269523	0.376186	0.426310
H	1.086276	−0.068594	−1.688383
H	1.463538	1.453636	−0.896874
O	0.833626	0.695500	1.564641
H	1.644815	0.290105	1.880865
H	−0.125022	−1.643117	1.539027
H	1.122184	−2.034917	0.355418
H	−1.460862	−2.689412	−0.189938
H	−0.472595	−1.993998	−1.472611
S	−2.293973	0.073973	1.071286
H	−2.435329	−0.409917	−1.355890
C	−1.062397	1.975788	−0.621223
H	−0.550210	2.039739	−1.582145
H	−2.110016	2.226357	−0.771191
H	−0.623771	2.709475	0.055055

Table S113: M06-2X optimized geometry of cis-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	0.405520	0.098824	0.699368
C	−0.695700	0.623628	−0.239987
C	−1.379902	−0.536067	−0.843633
C	−0.719292	−1.819323	−0.381465
C	0.086854	−1.406853	0.857743
H	0.996718	−1.992621	0.981140
H	−0.511184	−1.538330	1.757152
H	−0.066153	−2.175071	−1.180035
H	−1.442596	−2.604971	−0.170235
S	−2.379008	0.316489	0.422619
H	−1.785092	−0.467914	−1.844959
C	−0.499538	1.933806	−0.951251
H	−1.390492	2.192800	−1.519100
H	−0.306099	2.726031	−0.227907
H	0.349219	1.882004	−1.634762
O	0.411467	0.784371	1.936073
H	−0.477839	0.725140	2.303449
C	1.798163	0.341424	0.116359
C	2.084725	−0.372926	−1.198626
H	1.334539	−0.149435	−1.959315
H	3.053627	−0.068437	−1.591161
H	2.111497	−1.454409	−1.066790
H	1.933660	1.417981	0.005961
H	2.510707	0.017906	0.876873

Table S114: M06-2X optimized geometry of trans-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.466940	−0.006116	0.141286
C	0.891394	0.651048	−0.135402
C	1.918577	−0.410656	−0.050091
C	1.251171	−1.725747	0.292221
C	−0.218314	−1.506811	−0.090099
H	−0.898322	−2.111063	0.510019
H	−0.384338	−1.753384	−1.137113
H	1.345365	−1.881365	1.368697
H	1.699544	−2.577160	−0.216296
S	1.627673	0.203596	−1.741073
H	2.898121	−0.182192	0.347785
C	1.124778	2.050027	0.364243
H	2.157286	2.342140	0.183098
H	0.476879	2.759361	−0.150538
H	0.912427	2.100683	1.431166
C	−1.606258	0.575197	−0.685459
C	−2.953261	−0.083581	−0.410859
H	−2.924052	−1.152526	−0.624598
H	−3.264088	0.049568	0.627174
H	−3.731987	0.356181	−1.031875
H	−1.669206	1.644681	−0.474131
H	−1.346588	0.463826	−1.739407
O	−0.675332	0.235567	1.536764
H	−1.466137	−0.235771	1.811248

Table S115: M06-2X optimized geometry of cis-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (not H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−0.470879	−0.221282	0.059249
C	0.004565	−1.391045	−0.718593
C	1.450433	−1.170126	−1.123579
C	1.946858	−0.099935	−0.144357
C	0.705845	0.757468	0.168242
C	0.560945	1.879938	−0.858796
H	1.447909	2.515642	−0.828180
H	0.469742	1.480490	−1.870197
H	−0.310328	2.494712	−0.642409
O	0.718232	1.303913	1.475769
H	1.407643	1.971225	1.527502
H	2.287727	−0.558076	0.780674
H	2.758496	0.499853	−0.555603
H	2.041661	−2.083546	−1.088853
H	1.471715	−0.798471	−2.151326
S	−0.253784	−1.738508	1.043838
H	−0.666033	−1.908404	−1.392102
C	−1.859740	0.367204	−0.070074
C	−3.007844	−0.630109	−0.025312
H	−3.082041	−1.101042	0.951821
H	−3.948433	−0.124231	−0.239590
H	−2.877864	−1.422122	−0.763753
H	−1.980348	1.110109	0.721640
H	−1.897886	0.910959	−1.017651

Table S116: M06-2X optimized geometry of cis-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (H-bonded) (in Å) with the aTZ basis set

Atom	x	y	z
C	−1.856495	0.007932	0.573463
C	−0.381334	−0.315319	0.442166
C	0.121453	−1.575717	−0.140197
C	1.375276	−1.292975	−0.944579
C	1.886375	0.036057	−0.380900
C	0.628462	0.797616	0.093189
C	0.104783	1.704242	−1.010087
H	−0.816466	2.198123	−0.706036
H	0.853524	2.469485	−1.209579
H	−0.074188	1.140970	−1.926153
O	0.880650	1.648033	1.192615
H	1.161436	1.093077	1.929213
H	2.534838	−0.141519	0.474393
H	2.446983	0.617115	−1.110588
H	2.108955	−2.094474	−0.880827
H	1.087445	−1.186598	−1.993894
S	0.314702	−1.491825	1.670759
H	−0.569776	−2.338130	−0.473853
H	−2.298571	−0.688046	1.284045
H	−1.946798	1.003097	1.014256
C	−2.637017	−0.073437	−0.738822
H	−2.284663	0.640414	−1.479394
H	−2.561451	−1.071275	−1.171564
H	−3.692309	0.128460	−0.558180

Table S117: M06-2X optimized geometry of trans-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (in Å) with the aTZ basis set

Atom	x	y	z
C	−1.856495	0.007932	0.573463
C	−0.381334	−0.315319	0.442166
C	0.121453	−1.575717	−0.140197
C	1.375276	−1.292975	−0.944579
C	1.886375	0.036057	−0.380900
C	0.628462	0.797616	0.093189
C	0.104783	1.704242	−1.010087
H	−0.816466	2.198123	−0.706036
H	0.853524	2.469485	−1.209579
H	−0.074188	1.140970	−1.926153
O	0.880650	1.648033	1.192615
H	1.161436	1.093077	1.929213
H	2.534838	−0.141519	0.474393
H	2.446983	0.617115	−1.110588
H	2.108955	−2.094474	−0.880827
H	1.087445	−1.186598	−1.993894
S	0.314702	−1.491825	1.670759
H	−0.569776	−2.338130	−0.473853
H	−2.298571	−0.688046	1.284045
H	−1.946798	1.003097	1.014256
C	−2.637017	−0.073437	−0.738822
H	−2.284663	0.640414	−1.479394
H	−2.561451	−1.071275	−1.171564
H	−3.692309	0.128460	−0.558180

Table S118: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
128.9	0.8
186.1	2.7
210.8	95.1
213.6	1.1
240.6	5.0
267.9	0.4
312.3	0.7
363.2	1.8
380.4	2.5
422.6	1.6
481.6	12.6
534.8	13.2
587.4	6.0
661.6	1.6
691.2	4.0
812.5	3.5
853.1	7.1
893.5	17.2
944.2	6.4
949.6	2.8
955.4	9.4
994.2	1.9
1011.3	6.2
1045.3	7.8
1087.0	15.1
1101.5	61.3
1127.3	12.2
1168.3	18.2
1210.0	12.1
1226.3	37.4
1241.5	28.4
1258.7	24.0
1304.6	6.7
1333.0	3.9
1343.0	11.0
1400.3	10.8
1404.7	11.6
1412.5	8.7
1474.1	4.8
1484.5	7.0
1490.1	7.0
1495.4	10.6
1499.9	3.4
1507.8	8.2
1520.8	5.3
3054.7	11.5
3070.2	15.4
3071.8	20.3
3090.9	26.0
3117.5	16.1
3122.0	22.1
3138.4	11.8
3147.0	10.7
3150.7	10.8
3155.1	10.5
3176.0	19.4
3867.8	34.6

Table S119: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
112.9	3.0
196.1	0.1
213.9	1.3
232.4	1.3
266.9	0.7
308.8	0.7
354.9	4.5
373.1	3.4
413.6	49.1
434.3	32.9
482.3	26.6
539.5	14.2
594.3	5.3
665.0	2.5
687.2	4.4
809.9	0.6
846.1	5.8
895.7	14.9
943.8	8.3
951.8	4.3
962.7	5.6
994.8	14.9
1014.6	8.4
1046.2	28.1
1083.4	13.5
1116.7	5.9
1126.0	24.4
1169.7	38.0
1182.6	2.5
1227.1	51.2
1246.6	9.0
1294.5	18.2
1313.8	1.9
1335.9	2.9
1351.7	0.8
1387.7	38.3
1411.0	11.4
1426.7	30.3
1476.4	3.6
1483.3	7.5
1487.3	9.4
1494.2	10.3
1499.7	3.2
1509.3	4.7
1522.1	4.6
3065.5	8.2
3068.2	14.8
3073.4	21.9
3097.0	15.1
3118.3	18.4
3136.5	12.4
3140.7	9.9
3144.9	14.2
3150.5	19.9
3155.2	7.6
3180.0	18.4
3840.1	34.8

Table S120: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of trans-2,3-epoxy-1,2-dimethylcyclopentan-1-ol

Frequency	IR Intensity
118.3	2.3
184.2	0.6
223.9	4.8
242.5	1.8
264.3	0.3
270.0	38.8
281.4	61.4
354.0	1.6
381.7	8.1
425.1	1.2
481.7	14.7
513.7	1.8
600.2	2.3
654.7	1.3
702.1	2.1
813.9	3.9
854.2	4.4
887.5	8.7
937.0	3.7
951.5	22.1
959.1	13.6
992.7	2.1
1016.7	6.0
1041.9	6.6
1090.7	5.6
1094.8	84.9
1125.3	12.0
1164.4	1.4
1209.5	5.1
1228.6	69.3
1240.3	12.3
1257.6	3.7
1302.8	5.4
1339.0	5.3
1351.2	3.2
1401.5	2.6
1405.5	18.8
1415.3	20.3
1474.2	2.5
1483.3	5.9
1487.2	14.0
1492.0	4.8
1495.4	6.5
1506.3	2.0
1520.2	7.3
3053.0	15.9
3068.3	16.4
3081.9	24.7
3092.2	25.5
3122.4	13.1
3124.3	12.1
3136.9	11.3
3142.3	6.7
3146.7	21.8
3162.8	5.4
3183.9	18.4
3869.3	34.5

Table S121: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
72.9	0.4
122.6	0.9
171.5	8.5
198.3	56.3
205.0	19.6
224.0	9.4
270.4	19.7
285.5	1.5
321.9	1.2
356.1	1.3
392.3	2.9
423.4	4.3
484.1	10.0
545.8	12.1
590.8	5.0
662.5	1.8
707.4	2.5
791.8	1.0
803.6	5.4
853.4	7.3
893.8	16.7
944.8	1.0
950.6	16.0
980.9	6.8
1003.4	17.6
1030.7	1.9
1036.9	14.5
1051.6	19.5
1091.8	16.0
1104.7	19.7
1125.0	17.1
1165.1	15.6
1194.7	9.2
1233.2	57.2
1237.4	5.1
1248.9	20.5
1300.7	1.3
1318.5	2.6
1333.5	5.0
1344.5	9.5
1365.8	5.1
1399.3	8.0
1409.7	5.9
1421.5	5.7
1474.9	1.4
1483.7	11.0
1484.0	8.3
1495.2	9.3
1498.1	4.4
1505.8	5.9
1516.1	8.9
1518.6	6.5
3056.8	11.3
3066.4	19.0
3070.9	16.1
3072.7	23.0
3102.2	18.3
3105.6	11.0
3118.2	15.1
3132.2	22.4
3138.3	24.7
3142.4	11.5
3154.8	11.6
3155.5	12.8
3177.5	20.5
3876.1	33.1

Table S122: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
132.2	1.7
143.4	1.2
197.7	0.3
224.0	0.4
244.3	0.7
257.6	1.8
264.5	1.3
313.0	1.0
373.7	5.1
402.3	5.0
432.6	49.9
453.8	20.4
483.9	37.2
533.1	9.5
615.9	5.2
651.0	0.7
691.0	5.6
789.4	0.4
821.1	0.8
842.2	5.3
894.6	13.2
941.4	3.0
946.8	23.5
977.0	13.4
1006.1	1.2
1025.6	13.4
1053.5	23.5
1074.5	18.3
1087.1	18.6
1122.1	3.6
1130.5	32.8
1169.2	22.1
1182.4	8.6
1202.7	35.6
1246.3	1.3
1271.5	3.9
1293.7	9.2
1326.0	2.9
1335.7	5.7
1344.8	2.6
1382.1	21.2
1408.6	25.3
1410.4	13.5
1418.9	4.0
1475.6	3.9
1482.9	10.7
1493.2	12.7
1497.2	3.4
1500.4	2.1
1507.5	10.7
1517.1	5.5
1521.6	7.7
3062.4	9.4
3066.7	10.6
3070.5	23.2
3079.3	25.8
3095.6	16.9
3104.0	2.5
3118.4	14.6
3129.6	31.8
3134.9	8.0
3139.2	33.0
3142.3	11.8
3154.0	9.2
3176.4	18.0
3837.8	35.4

Table S123: Frequencies and IR Intensities of trans-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol.

Frequency	IR Intensity
99.5	0.2
117.2	2.2
169.7	1.2
192.8	1.1
237.3	8.0
246.4	3.9
272.4	49.2
275.3	48.1
302.2	3.3
362.0	1.8
404.6	3.3
436.8	3.7
489.8	11.7
521.3	2.3
588.2	1.6
677.7	0.6
705.2	2.4
786.9	4.2
825.7	3.1
850.7	6.6
894.1	10.2
945.5	4.9
966.7	20.6
982.5	7.2
991.1	24.8
1024.9	27.7
1033.4	1.5
1047.8	2.5
1092.1	5.5
1100.0	38.0
1126.1	17.4
1166.4	1.8
1204.6	2.4
1224.2	66.2
1239.3	5.3
1248.2	9.2
1301.3	5.3
1319.0	5.5
1335.9	7.1
1349.8	1.8
1360.9	3.3
1404.2	14.1
1410.6	3.8
1426.8	15.6
1475.5	2.2
1482.6	8.2
1485.4	5.7
1492.9	3.7
1493.7	7.8
1504.8	7.8
1513.2	5.1
1521.0	8.2
3056.4	12.7
3062.9	17.4
3069.6	20.6
3080.7	26.8
3089.7	20.1
3100.8	2.4
3122.4	7.9
3123.9	29.6
3137.4	8.1
3138.3	26.7
3140.5	18.9
3162.4	5.5
3183.8	19.6
3875.3	31.0

Table S124: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
85.6	0.3
116.6	1.1
184.8	6.5
192.6	66.9
201.7	25.5
233.5	1.1
276.6	2.3
303.8	1.3
320.7	0.9
364.3	1.7
405.2	3.0
442.8	2.7
486.6	13.1
556.0	4.0
599.9	15.8
650.7	1.9
697.3	2.0
773.6	2.5
815.2	3.9
869.4	11.5
922.3	5.3
947.8	2.5
957.7	16.3
968.0	7.2
981.4	10.9
1016.2	8.7
1025.4	18.5
1058.3	4.7
1090.0	14.8
1112.1	36.6
1122.6	5.5
1167.0	26.2
1209.6	7.9
1217.0	42.3
1239.5	14.4
1243.1	27.5
1293.2	8.2
1308.9	1.1
1332.0	6.6
1341.5	11.1
1370.6	1.3
1404.7	17.4
1409.2	0.7
1413.2	6.7
1478.5	7.2
1483.7	0.6
1494.1	7.3
1498.1	9.9
1499.8	8.8
1503.8	0.8
1509.4	10.3
1514.9	7.3
3052.8	11.0
3068.4	17.6
3072.7	25.8
3073.4	11.0
3090.7	25.5
3114.8	0.5
3117.6	15.6
3120.9	31.4
3135.2	24.4
3141.9	17.7
3146.3	17.8
3150.5	10.4
3177.5	19.1
3868.6	34.6

Table S125: Frequencies and IR Intensities of cis-2-ethyl-2,3-epoxy-1-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
95.8	1.0
105.0	1.9
173.5	0.4
201.8	0.2
228.7	2.3
273.6	0.3
300.7	1.7
318.7	1.0
359.5	2.7
396.4	27.7
415.1	58.2
442.8	4.9
485.0	26.6
558.7	5.9
605.4	12.1
654.5	3.7
693.8	2.8
776.2	2.8
814.9	1.2
864.2	7.9
925.6	1.3
949.9	2.0
956.8	19.9
967.9	5.8
980.2	14.6
1017.9	28.3
1027.2	13.1
1059.3	22.3
1091.1	5.9
1112.1	7.7
1126.2	11.9
1171.6	32.6
1181.0	2.1
1225.2	50.0
1240.9	12.6
1267.3	1.3
1299.5	14.5
1316.0	8.2
1335.8	2.1
1350.5	0.2
1372.2	6.7
1391.4	27.7
1413.2	5.9
1425.8	32.1
1480.1	9.4
1481.6	2.4
1490.3	4.9
1498.4	15.0
1499.1	3.0
1505.9	0.6
1511.5	7.0
1516.4	5.0
3063.5	7.1
3066.3	10.2
3070.9	23.1
3072.7	23.9
3097.9	15.1
3110.2	2.4
3118.2	19.1
3135.9	22.9
3140.1	16.6
3143.6	16.2
3146.6	32.5
3150.2	5.0
3176.0	18.3
3840.6	35.6

Table S126: Frequencies and IR Intensities of trans-2-ethyl-2,3-epoxy-1-methylcyclopentan-1-ol

Frequency	IR Intensity
40.6	0.0
119.0	1.9
175.0	1.3
214.5	1.4
226.8	3.9
259.4	0.9
272.0	47.7
276.4	46.7
306.3	1.5
377.4	8.3
396.0	3.9
432.9	1.8
482.8	14.4
554.3	5.4
596.7	2.6
647.3	2.8
705.5	0.2
776.5	3.2
818.2	1.9
871.0	5.7
910.0	2.0
940.4	4.2
957.9	6.4
970.9	31.4
998.6	3.8
1008.6	21.2
1028.2	15.4
1063.7	11.7
1091.2	22.5
1103.5	37.4
1127.5	4.5
1163.9	1.8
1207.3	5.5
1224.4	49.6
1238.6	19.6
1242.9	10.0
1292.3	5.2
1314.0	7.4
1336.0	6.8
1351.1	3.1
1368.1	1.4
1403.5	8.4
1410.6	1.2
1419.4	22.3
1473.6	3.1
1485.0	4.5
1491.6	4.3
1496.5	7.0
1497.4	12.5
1500.2	5.2
1506.2	1.5
1518.9	6.3
3053.5	14.4
3062.6	16.9
3069.2	29.1
3079.6	24.5
3090.9	25.4
3104.1	11.9
3122.3	7.0
3123.3	18
3131.5	31.4
3142.8	8.5
3148.7	19.0
3168.3	8.0
3178.5	17.7
3865.4	32.8

Table S127: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
132.6	1.3
167.5	97.5
194.9	2.4
218.0	4.1
243.1	0.8
275.7	1.0
327.9	0.7
367.4	1.9
382.5	1.4
426.2	5.1
481.4	7.9
522.6	17.3
587.0	4.2
655.7	1.6
671.8	2.4
812.4	2.0
854.4	0.6
873.7	26.0
930.5	5.6
948.8	7.5
956.8	13.6
976.5	5.5
1005.1	9.1
1017.3	34.6
1053.2	24.1
1091.1	21.9
1093.9	13.3
1128.2	31.0
1152.9	25.7
1165.0	14.7
1209.4	19.4
1240.1	23.9
1246.1	18.4
1294.1	16.5
1315.7	18.3
1338.3	1.5
1353.5	9.6
1403.1	23.1
1410.5	4.6
1417.4	4.4
1469.5	6.5
1482.7	5.0
1489.2	9.3
1492.9	7.4
1500.3	4.0
1504.1	6.5
1518.2	0.7
3054.6	12.6
3059.9	20.7
3069.8	27.9
3088.8	30.9
3114.0	19.4
3121.8	23.8
3128.6	13.7
3133.0	14.8
3146.4	15.9
3152.3	10.1
3183.6	16.1
3544.4	3.5
3869.9	31.8

Table S128: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
118.3	2.2
210.7	0.0
219.3	0.3
230.0	1.0
272.7	0.7
320.4	1.0
355.5	5.7
377.2	2.0
424.3	13.7
446.9	55.7
482.4	31.3
527.9	16.3
594.3	4.1
660.5	8.5
668.8	1.0
813.1	0.2
846.7	0.4
877.8	15.2
930.9	10.0
947.2	11.1
961.2	9.3
980.7	1.8
1007.9	10.8
1023.4	57.0
1054.7	24.9
1090.4	4.9
1110.4	8.4
1132.7	21.5
1136.9	10.5
1180.9	2.1
1202.3	18.2
1232.1	82.7
1252.0	0.5
1304.4	9.9
1337.8	3.8
1352.0	0.6
1358.7	4.9
1392.7	34.9
1414.6	9.6
1428.8	39.4
1472.8	4.7
1483.9	7.2
1488.2	7.3
1490.4	8.4
1501.5	2.2
1504.1	7.0
1519.7	1.0
3056.8	19.4
3063.9	11.3
3070.3	28.8
3096.7	17.1
3114.3	20.8
3124.9	12.9
3132.4	12.6
3138.6	17.3
3144.4	17.9
3149.7	16.1
3186.0	15.6
3540.5	3.8
3828.6	32.0

Table S129: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of trans-2,3- aziridine-1,2-dimethylcyclopentan-1-ol

Frequency	IR Intensity
124.9	1.4
199.6	0.3
227.7	6.5
245.1	1.9
256.4	85.8
259.0	3.2
286.4	9.2
352.4	1.1
385.7	8.9
432.2	0.4
476.6	17.4
501.8	1.7
600.5	4.5
649.0	0.1
685.0	0.2
815.4	3.0
853.6	1.7
873.2	15.3
925.1	6.8
946.1	15.5
956.5	11.3
975.3	18.8
1005.1	10.5
1024.1	44.3
1049.3	36.2
1092.7	13.5
1098.7	15.3
1130.0	9.4
1143.3	6.2
1169.3	5.8
1209.8	6.5
1237.7	24.5
1246.3	62.6
1295.5	13.9
1315.4	9.7
1347.4	1.6
1358.1	2.9
1401.0	11.7
1409.1	11.6
1421.8	11.6
1473.2	3.4
1478.9	8.8
1484.7	8.0
1493.3	1.0
1495.0	6.8
1504.5	3.2
1513.6	3.7
3052.1	18.9
3056.2	25.0
3078.8	29.5
3088.5	32.2
3117.0	21.9
3120.8	12.1
3121.7	15.2
3142.7	3.7
3147.3	22.6
3152.0	5.9
3191.1	15.2
3541.8	3.5
3872.1	32.8

Table S130: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-aziridine-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
83.7	0.2
117.0	0.1
190.8	0.1
218.8	4.6
227.3	0.6
235.6	38.3
279.6	28.8
296.8	26.6
332.2	1.2
365.5	4.2
391.5	8.3
427.6	0.6
489.5	12.1
531.7	4.5
595.1	3.9
654.0	4.0
698.7	0.8
793.0	1.8
808.9	6.7
843.0	17.1
878.3	16.1
919.7	24.1
952.3	4.0
980.9	8.6
1007.3	11.2
1022.6	37.5
1028.2	5.5
1047.3	12.4
1082.8	14.7
1104.0	8.0
1115.1	40.8
1125.5	5.7
1131.9	13.3
1186.9	5.6
1203.5	2.0
1229.8	49.9
1251.7	3.4
1280.9	51.3
1306.2	2.5
1323.6	3.3
1334.6	13.5
1341.5	0.4
1365.1	4.2
1400.4	12.5
1409.5	5.2
1420.9	3.0
1469.8	5.2
1481.7	10.2
1495.0	6.1
1500.0	9.0
1504.0	4.4
1507.4	4.6
1512.3	0.2
1520.5	10.7
3057.3	7.5
3063.7	16.6
3064.3	26.5
3067.2	32.9
3088.6	10.6
3105.8	24.7
3110.4	1.9
3128.1	25.0
3132.1	1.4
3134.6	37.3
3143.2	23.0
3153.1	11.5
3179.0	20.6
3543.3	3.3
3872.9	31.3

Table S131: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-aziridine-1-ethyl-2-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
139.3	1.3
152.1	0.3
201.7	0.4
221.8	0.3
252.1	0.7
266.6	1.6
269.2	0.3
328.5	0.6
377.4	3.8
406.7	7.1
443.3	10.3
464.3	18.9
495.4	70.6
522.2	10.9
616.2	4.5
647.9	3.3
671.9	4.3
791.7	0.5
824.2	1.4
843.0	1.2
877.2	13.6
930.8	14.0
948.1	8.1
971.5	32.9
984.5	2.9
1020.0	16.2
1036.1	27.0
1053.5	30.3
1076.0	19.8
1094.3	5.0
1119.2	5.7
1130.4	29.0
1142.4	13.0
1174.6	3.3
1198.8	6.2
1209.4	56.1
1251.8	4.8
1288.2	1.6
1305.0	5.5
1333.3	1.2
1343.6	8.9
1358.6	5.3
1387.8	15.2
1412.1	13.2
1415.5	26.6
1421.0	12.9
1473.0	7.0
1484.1	7.4
1488.5	8.7
1497.0	6.1
1500.5	3.9
1506.4	10.7
1512.9	5.1
1522.1	3.3
3056.4	18.9
3062.2	10.2
3069.8	21.0
3076.2	33.2
3094.4	19.3
3103.0	3.4
3115.5	18.7
3124.0	10.7
3128.5	41.0
3133.9	7.8
3137.4	32.9
3142.8	15.4
3184.4	14.8
3538.5	3.9
3822.8	33.8

Table S132: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of trans-2,3-aziridine-1-ethyl-2-methylcyclopentan-1-ol

Frequency	IR Intensity
97.7	0.2
115.1	1.0
172.6	0.5
193.2	0.7
237.7	10.6
242.2	0.9
283.2	80.2
285.6	4.5
307.2	10.7
362.7	4.0
416.1	3.9
442.8	6.7
489.6	3.0
499.2	1.9
588.0	1.2
667.6	5.9
696.8	5.1
784.5	2.8
830.8	5.9
833.4	19.9
883.1	10.1
920.0	23.1
961.7	17.6
984.6	2.9
989.3	28.5
1016.7	11.1
1028.3	20.7
1040.7	7.9
1085.4	27.5
1091.3	14.3
1111.5	19.3
1118.7	1.2
1132.4	1.8
1190.4	4.6
1213.3	44.4
1222.0	25.6
1241.7	3.5
1271.2	12.9
1316.1	11.0
1318.1	3.2
1335.3	8.0
1342.6	4.6
1361.2	0.9
1403.5	15.4
1408.5	4.4
1421.5	12.4
1471.9	3.5
1481.8	5.0
1488.1	6.7
1492.3	2.1
1502.2	9.0
1504.3	6.2
1506.8	4.6
1514.4	5.1
3056.5	2.9
3060.6	28.2
3066.5	24.5
3071.8	26.4
3077.5	24.2
3099.1	4.9
3112.2	7.1
3123.8	31.8
3125.1	28.2
3134.2	11.4
3137.7	25.8
3161.6	6.7
3186.6	18.9
3532.6	0.9
3874.3	27.6

Table S133: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-aziridine-1-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
91.4	0.5
109.5	0.3
180.9	0.7
207.5	2.0
244.1	4.6
251.9	78.7
281.3	6.9
299.9	5.9
347.7	0.4
372.3	3.1
419.7	1.2
441.8	4.3
485.5	11.3
546.8	2.3
598.3	6.2
645.6	2.6
685.9	0.9
773.3	6.8
820.0	4.4
858.5	20.1
898.6	1.8
928.7	35.3
947.7	4.8
966.1	14.9
987.2	7.3
1000.4	22.6
1026.3	3.3
1056.9	2.0
1088.2	16.0
1103.2	7.8
1117.8	50.3
1120.9	22.1
1136.3	9.6
1192.8	6.9
1209.1	2.8
1227.9	71.4
1245.4	4.6
1261.3	9.5
1306.2	21.4
1321.5	4.8
1326.9	12.4
1339.3	3.0
1370.3	6.3
1405.6	4.8
1407.4	15.7
1411.6	8.5
1463.7	5.6
1486.0	2.8
1494.2	2.1
1497.3	3.6
1501.8	9.5
1510.1	5.3
1514.0	2.8
1517.2	10.5
3051.0	13.4
3063.5	14.5
3067.1	25.5
3068.1	28.5
3084.2	16.2
3105.1	18.1
3113.6	0.6
3118.5	31.5
3127.6	22.3
3130.9	25.7
3145.4	25.4
3147.8	11.5
3180.5	18.1
3540.5	3.3
3866.5	33.2

Table S134: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-aziridine-1-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
96.8	0.6
108.6	1.1
174.7	0.4
210.3	0.3
241.3	1.0
276.5	0.3
301.1	2.4
337.2	0.5
364.5	2.3
409.0	3.4
440.3	2.8
464.5	33.2
493.4	71.7
547.7	5.9
603.6	6.2
652.4	8.4
676.5	3.9
772.7	3.4
816.5	1.1
863.3	1.9
889.8	11.4
941.3	22.7
948.2	15.0
967.8	12.7
984.0	2.2
1011.3	3.6
1021.8	21.1
1030.0	38.2
1073.6	20.3
1096.8	3.8
1108.7	11.3
1123.7	5.2
1139.9	13.4
1177.0	5.5
1200.7	19.4
1232.0	84.7
1249.2	0.8
1272.7	0.3
1314.1	10.9
1335.8	7.3
1349.5	1.5
1363.3	10.7
1373.5	5.0
1399.5	24.6
1413.6	6.5
1430.5	45.8
1471.1	4.8
1481.9	3.5
1487.1	4.8
1490.0	9.0
1499.8	7.1
1504.8	2.5
1511.0	3.5
1515.5	3.9
3052.6	20.8
3063.9	9.3
3068.6	26.0
3070.4	26.3
3089.0	9.2
3097.7	17.5
3114.0	22.9
3133.1	25.3
3140.2	18.1
3143.5	14.6
3146.8	23.3
3156.8	12.5
3183.6	15.3
3538.8	3.8
3823.9	33.1

Table S135: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of trans-2-ethyl-2,3-aziridine-1-methylcyclopentan-1-ol

Frequency	IR Intensity
45.7	0.1
122.0	1.0
182.8	0.7
228.0	0.3
234.8	4.5
262.7	0.6
268.5	0.3
305.7	70.0
311.0	19.3
382.1	13.0
402.7	5.5
438.8	0.3
476.9	16.6
541.1	4.0
598.1	4.5
642.7	0.9
690.5	0.8
771.2	3.6
818.3	3.4
868.7	2.7
885.4	13.4
930.9	13.1
947.6	25.5
964.9	30.4
988.9	1.1
1004.9	6.1
1023.4	25.2
1031.7	22.5
1077.5	15.5
1096.7	23.5
1105.5	12.3
1124.5	3.0
1138.0	1.6
1168.5	7.0
1208.0	7.0
1237.4	15.9
1243.8	76.6
1265.2	0.6
1312.3	11.7
1323.3	12.6
1348.8	4.3
1357.1	2.6
1369.8	3.4
1400.7	13.7
1412.8	7.9
1428.7	11.9
1468.1	3.0
1479.4	7.4
1481.0	2.7
1494.0	2.8
1495.5	4.9
1499.3	4.2
1504.2	4.8
1516.8	4.8
3047.3	25.4
3052.6	19.2
3068.1	27.1
3077.4	29.2
3084.9	18.8
3088.6	35.0
3120.5	8.7
3121.0	21.7
3128.6	33.2
3144.6	4.7
3149.2	21.4
3175.3	6.2
3187.0	14.8
3544.3	3.5
3866.5	30.8

Table S136: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
119.3	0.1
206.6	1.9
211.9	1.7
236.2	12.5
253.7	77.6
278.2	1.2
308.8	0.8
324.0	5.8
355.0	0.0
383.2	0.9
428.9	3.5
481.7	10.3
559.9	1.7
595.7	0.2
607.7	0.9
651.1	1.5
715.5	1.7
765.8	1.5
837.1	4.2
893.3	8.1
921.4	9.4
945.2	8.4
957.5	1.2
977.6	0.2
989.2	7.2
1013.7	8.3
1052.4	3.9
1085.7	19.3
1104.3	27.0
1140.4	22.5
1175.6	32.1
1203.4	8.5
1233.9	49.7
1236.8	8.4
1261.4	4.3
1322.8	18.3
1329.9	13.6
1366.1	2.2
1393.9	24.1
1403.0	9.6
1412.0	4.2
1487.9	2.2
1489.7	2.7
1496.1	8.8
1499.2	12.4
1509.7	5.0
1516.3	1.5
2432.2	75.1
3052.8	14.2
3054.8	27.4
3058.4	34.2
3080.6	12.9
3113.6	19.6
3116.5	13.7
3122.0	20.8
3128.5	25.3
3142.5	11.3
3150.6	12.4
3194.0	5.1
3867.3	32.8

Table S137: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
119.3	0.1
206.6	1.9
211.9	1.7
236.2	12.5
253.7	77.6
278.2	1.2
308.8	0.8
324.0	5.8
355.0	0.0
383.2	0.9
428.9	3.5
481.7	10.3
559.9	1.7
595.7	0.2
607.7	0.9
651.1	1.5
715.5	1.7
765.8	1.5
837.1	4.2
893.3	8.1
921.4	9.4
945.2	8.4
957.5	1.2
977.6	0.2
989.2	7.2
1013.7	8.3
1052.4	3.9
1085.7	19.3
1104.3	27.0
1140.4	22.5
1175.6	32.1
1203.4	8.5
1233.9	49.7
1236.8	8.4
1261.4	4.3
1322.8	18.3
1329.9	13.6
1366.1	2.2
1393.9	24.1
1403.0	9.6
1412.0	4.2
1487.9	2.2
1489.7	2.7
1496.1	8.8
1499.2	12.4
1509.7	5.0
1516.3	1.5
2432.2	75.1
3052.8	14.2
3054.8	27.4
3058.4	34.2
3080.6	12.9
3113.6	19.6
3116.5	13.7
3122.0	20.8
3128.5	25.3
3142.5	11.3
3150.6	12.4
3194.0	5.1
3867.3	32.8

Table S138: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of trans-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol

Frequency	IR Intensity
119.0	0.7
194.7	0.2
217.5	3.5
236.9	21.5
243.6	9.7
254.2	61.8
293.7	2.2
319.2	1.0
330.4	4.1
390	6.3
410.5	2.5
457.5	2.1
561.5	2.5
608.3	1.5
611.0	3.2
653.2	12.4
723.8	2.2
783.5	3.5
825.6	6.7
893.2	7.8
910.6	5.0
945.2	0.8
954.2	23.7
979.1	12.9
988.4	2.3
1018.7	6.0
1055.1	3.6
1081.2	64.4
1095.6	0.5
1138.9	2.3
1177.4	29.6
1206.6	5.0
1225.5	0.2
1237.8	15.8
1257.3	31.8
1322.2	4.5
1341.5	3.5
1365.6	7.3
1393.5	11.0
1408.5	17.5
1412.4	11.9
1484.4	1.4
1486.4	8.6
1493.5	2.0
1498.8	3.1
1500.0	7.4
1504.0	8.5
2437.7	69.3
3054.4	18.3
3062.3	26.2
3074.7	26.9
3075.6	14.3
3116.9	15.7
3123.1	19.8
3127.6	21.2
3128.4	14.1
3141.5	8.2
3147.4	13.2
3197.4	4.1
3866.5	31.9

Table S139: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
58.0	0.1
119.8	0.0
178.1	0.6
213.0	52.3
217.4	2.1
226.8	23.2
273.8	15.0
289.9	5.7
316.1	2.2
340.9	4.9
351.0	1.9
372.8	0.4
428.6	4.3
507.1	7.9
559.6	1.7
594.3	0.7
634.7	1.7
662.6	1.4
727.9	1.7
744.1	0.8
793.8	1.8
840.8	4.5
903.1	8.3
924.3	11.1
943.8	5.2
960.7	4.8
984.4	6.4
1011.6	16.2
1020.3	2.2
1044.2	17.5
1060.4	8.2
1085.8	7.9
1108.6	15.3
1140.2	18.9
1174.4	15.6
1191.4	9.3
1230.5	43.9
1233.6	9.2
1265.6	3.5
1308.2	16.4
1314.2	15.4
1331.6	0.7
1359.1	9.3
1373.2	0.5
1397.7	19.4
1411.2	4.1
1420.6	5.1
1478.4	2.8
1496.0	10.0
1497.1	6.0
1502.9	6.8
1506.7	4.3
1509.1	3.6
1519.1	12.9
2436.3	76.1
3054.5	23.7
3056.7	19.0
3061.1	17.1
3064.8	32.3
3087.6	9.2
3109.6	11.1
3114.7	16.1
3119.2	14.1
3127.4	15.7
3135.6	27.4
3141.9	14.7
3147.4	28.3
3192.7	5.3
3874.8	31.2

Table S140: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
130.0	0.9
155.4	0.2
217.4	0.1
226.4	0.1
233.1	0.4
257.1	0.3
290.0	0.1
314.6	0.8
328.6	3.4
357.2	7.9
370.9	67.2
415.0	4.5
446.2	11.1
475.9	5.6
563.7	2.9
599.0	2.4
601.8	2.2
651.3	2.4
712.2	1.9
747.7	2.3
797.5	2.8
834.8	0.4
890.6	8.6
928.4	4.3
938.4	8.7
961.4	3.3
982.7	10.1
1009.1	7.6
1037.4	17.4
1056.5	6.7
1074.8	29.2
1087.2	10.5
1110.9	14.5
1142.2	20.7
1172.0	7.4
1194.5	24.6
1222.4	23.2
1241.0	6.8
1250.9	5.9
1308.4	3.1
1324.6	1.3
1329.4	2.2
1370.7	41.3
1386.5	12.9
1393.8	23.3
1413.4	11.7
1418.1	2.9
1485.1	0.2
1491.7	9.9
1494.7	14.0
1502.3	2.9
1506.8	15.5
1511.6	2.8
1524.1	3.4
2443.4	62.7
3055.8	21.3
3063.3	12.1
3073.4	15.8
3078.3	14.3
3080.9	31.4
3108.0	2.1
3117.1	18.5
3118.6	14.6
3128.4	22.7
3132.1	37.1
3138.6	19.1
3140.0	11.7
3189.8	3.9
3831.1	21.8

Table S141: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of trans-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol

Frequency	IR Intensity
130.0	0.9
155.4	0.2
217.4	0.1
226.4	0.1
233.1	0.4
257.1	0.3
290.0	0.1
314.6	0.8
328.6	3.4
357.2	7.9
370.9	67.2
415.0	4.5
446.2	11.1
475.9	5.6
563.7	2.9
599.0	2.4
601.8	2.2
651.3	2.4
712.2	1.9
747.7	2.3
797.5	2.8
834.8	0.4
890.6	8.6
928.4	4.3
938.4	8.7
961.4	3.3
982.7	10.1
1009.1	7.6
1037.4	17.4
1056.5	6.7
1074.8	29.2
1087.2	10.5
1110.9	14.5
1142.2	20.7
1172.0	7.4
1194.5	24.6
1222.4	23.2
1241.0	6.8
1250.9	5.9
1308.4	3.1
1324.6	1.3
1329.4	2.2
1370.7	41.3
1386.5	12.9
1393.8	23.3
1413.4	11.7
1418.1	2.9
1485.1	0.2
1491.7	9.9
1494.7	14.0
1502.3	2.9
1506.8	15.5
1511.6	2.8
1524.1	3.4
2443.4	62.7
3055.8	21.3
3063.3	12.1
3073.4	15.8
3078.3	14.3
3080.9	31.4
3108.0	2.1
3117.1	18.5
3118.6	14.6
3128.4	22.7
3132.1	37.1
3138.6	19.1
3140.0	11.7
3189.8	3.9
3831.1	21.8

Table S142: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
82.4	0.1
112.6	0.1
186.9	1.0
208.5	1.5
232.1	2.3
246.5	83.6
287.2	9.4
296.0	0.9
316.4	0.5
354.7	0.8
364.0	2.7
386.7	0.4
446.2	2.9
492.1	8.4
558.5	1.8
599.4	0.4
621.3	1.0
691.0	1.6
726.3	1.4
752.4	4.3
803.4	2.8
840.7	5.1
906.4	13.0
920.1	15.5
951.0	0.5
958.7	0.8
966.5	5.3
993.7	0.9
1014.9	7.6
1023.4	1.6
1065.2	1.7
1083.7	8.5
1108.8	26.6
1140.9	25.8
1173.9	30.5
1203.3	2.2
1209.3	24.9
1233.9	39.3
1256.5	6.0
1314.1	1.6
1318.4	15.8
1328.3	18.0
1358.7	1.5
1372.9	6.5
1391.8	19.4
1406.2	11.2
1410.6	8.1
1486.0	1.2
1492.5	1.9
1497.6	4.8
1506.1	14.6
1507.8	3.4
1511.9	1.3
1514.7	9.8
2426.5	74.2
3053.5	14.1
3057.4	33.1
3069.2	23.3
3072.7	14.0
3080.0	13.4
3111.2	5.8
3112.3	19.5
3122.2	26.7
3127.9	24.8
3130.0	25.6
3152.1	11.9
3155.3	19.7
3199.3	4.3
3867.9	32.5

Table S143: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
95.7	0.6
116.9	0.9
194.5	0.1
208.7	0.6
229.5	0.2
280.0	0.5
291.8	0.5
313.2	0.2
344.0	5.9
359.8	1.5
376.9	51.8
390.7	27.5
443.7	3.5
487.4	10.9
559.3	3.2
597.7	0.7
619.9	5.2
682.7	2.3
716.0	2.1
749.0	2.3
801.5	3.2
835.3	0.9
903.0	11.8
925.1	3.8
953.5	0.1
960.5	0.9
971.9	4.7
994.6	2.8
1017.0	35.8
1024.3	9.5
1064.6	2.5
1086.3	3.7
1104.8	11.6
1145.9	22.2
1167.3	7.8
1203.5	1.3
1227.0	39.0
1238.9	43.7
1246.5	10.9
1315.7	3.7
1324.4	13.2
1341.4	1.6
1360.5	2.8
1379.3	20.7
1382.3	37.0
1410.0	8.5
1417.2	29.4
1484.0	2.5
1489.2	4.4
1495.0	5.7
1504.6	14.5
1507.7	4.2
1509.9	0.9
1515.8	4.5
2447.7	62.8
3060.3	23.4
3068.4	10.3
3070.6	16.3
3071.3	24.7
3078.7	9.0
3109.4	5.7
3117.2	22.2
3130.7	23.5
3133.9	19.4
3144.5	24.0
3153.8	14.5
3159.4	13.3
3195.2	3.7
3831.2	21.6

Table S144: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of trans-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol

Frequency	IR Intensity
76.4	0.2
109.7	0.5
203.1	0.4
212.9	0.4
219.4	1.4
246.9	3.6
274.2	77.9
283.2	4.9
292.8	5.9
313.8	1.2
362.8	5.7
401.9	4.8
416.3	3.7
475.5	4.0
557.9	2.5
609.7	3.6
613.5	0.9
685.4	6.6
718.4	4.8
753.1	2.3
816.6	16.5
826.2	2.6
904.4	6.3
909.0	14.5
950.2	2.8
964.0	5.6
964.9	14.5
999.7	7.1
1011.5	4.4
1034.4	2.6
1063.5	1.1
1090.5	26.3
1099.4	23.4
1138.5	3.6
1174.4	23.8
1205.0	5.6
1206.0	3.2
1232.1	11.8
1253.7	34.1
1317.1	12.4
1318.1	3.5
1340.0	2.6
1359.5	0.9
1369.1	6.1
1390.4	9.1
1407.7	2.5
1412.6	31.8
1482.0	3.6
1484.2	3.9
1494.0	2.0
1497.1	4.7
1498.2	5.3
1501.8	8.5
1511.8	3.6
2439.5	67.2
3052.7	17.7
3068.1	31.0
3070.5	27.2
3072.3	17.5
3075.4	14.4
3106.7	11.1
3116.8	16.1
3121.6	17.7
3126.3	23.8
3127.3	30.7
3148.5	13.1
3171.0	8.1
3202.0	3.4
3862.4	29.7

Table S145: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-thiirane-1,2-dimethylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
123.1	0.3
205.3	53.8
214.0	1.3
218.1	38.1
242.3	5.4
278.3	0.8
328.4	2.1
333.7	0.8
358.6	0.3
383.5	0.9
434.6	6.0
497.5	12.0
573.1	3.4
618.9	1.1
629.3	2.6
678.3	15.0
774.0	1.0
835.5	6.2
914.2	2.6
943.0	4.7
950.3	2.2
984.5	0.9
990.5	8.4
1017.0	7.2
1058.9	1.8
1078.4	18.9
1102.2	35.9
1143.4	18.9
1187.2	34.7
1206.6	10.1
1236.7	1.6
1238.9	58.1
1267.8	1.8
1326.7	5.1
1333.1	19.5
1376.6	1.0
1397.6	30.6
1405.1	2.0
1414.6	6.1
1483.5	1.8
1489.2	11.7
1491.3	6.5
1497.9	10.9
1502.5	2.3
1514.5	0.9
3055.4	9.5
3060.5	25.2
3063.0	22.9
3093.2	22.7
3121.0	19.3
3123.1	18.0
3129.0	11.1
3150.1	9.3
3152.4	11.0
3155.4	8.4
3186.4	7.2
3869.9	36.6

Table S146: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-thiirane-1,2-dimethylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
122.5	2.6
216.7	0.5
223.1	0.3
232.7	0.1
273.3	0.8
323.6	0.7
326.7	0.6
352.5	1.1
378.9	2.6
416.5	61.2
436.9	29.0
502.0	18.6
572.2	6.9
612.1	0.5
630.1	5.7
673.4	11.4
767.4	1.2
831.8	3.1
913.9	0.2
946.7	2.8
958.8	1.6
985.6	8.9
992.1	4.0
1020.0	32.3
1057.9	9.3
1081.1	13.6
1103.2	6.4
1146.3	31.0
1168.5	6.6
1218.1	7.3
1241.6	44.8
1252.0	34.3
1271.9	1.0
1325.8	1.3
1346.1	7.6
1379.1	52.6
1397.6	15.0
1415.9	9.5
1419.9	16.5
1482.3	4.2
1485.0	3.7
1490.7	12.7
1496.2	8.3
1501.0	5.3
1515.7	0.4
3061.2	19.8
3062.8	12.5
3067.9	17.2
3100.7	11.5
3123.9	16.6
3129.1	9.0
3142.2	12.9
3146.7	14.2
3154.0	10.8
3156.6	11.0
3186.5	5.7
3825.4	25.2

Table S147: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of trans-2,3-thiirane-1,2-dimethylcyclopentan-1-ol

Frequency	IR Intensity
118.7	1.1
204.8	0.7
222.0	2.0
239.5	2.7
251.7	1.6
272.2	88.3
299.5	6.6
330.5	1.3
340.7	2.9
392.0	5.3
416.2	2.9
468.5	2.2
581.4	8.7
619.6	0.9
632.1	3.9
679.0	28.2
787.5	7.3
831.1	1.0
907.4	5.1
930.3	6.3
954.7	21.9
981.8	5.0
995.8	0.5
1017.9	6.6
1060.3	10.8
1078.4	52.2
1096.3	10.0
1142.2	1.5
1188.3	33.7
1209.5	9.5
1229.8	1.9
1237.0	12.9
1263.8	20.8
1327.5	4.2
1345.1	5.7
1377.8	10.0
1400.2	9.0
1409.5	24.3
1415.2	3.3
1477.3	4.2
1486.2	7.8
1491.3	4.3
1494.6	6.3
1500.0	7.0
1502.4	2.9
3055.4	17.0
3070.0	17.7
3074.2	20.7
3092.5	24.0
3124.4	14.1
3127.9	13.5
3138.3	10.2
3145.4	6.6
3150.1	15.3
3155.9	6.6
3193.0	5.6
3868.2	36.3

Table S148: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol ((not H-bonded)

Frequency	IR Intensity
67.5	0.3
122.9	0.3
180.0	1.1
208.5	66.7
221.1	1.8
227.6	11.2
278.2	23.7
288.2	1.1
328.9	1.9
349.5	1.4
352.2	1.4
369.6	0.7
430.8	7.7
520.6	7.5
571.2	3.3
622.5	3.5
651.0	1.2
679.5	17.1
752.0	1.6
796.3	2.3
836.3	5.9
913.9	2.8
940.0	4.4
960.7	6.1
990.3	8.2
1014.7	11.0
1021.3	5.9
1041.6	16.7
1068.5	8.0
1077.9	10.5
1107.0	16.5
1143.0	16.0
1183.1	14.2
1197.6	16.7
1231.4	20.5
1233.8	35.5
1271.0	1.7
1311.7	4.5
1324.1	15.6
1330.6	0.2
1363.0	7.7
1383.4	0.2
1399.6	20.6
1412.3	2.2
1422.4	8.4
1478.1	2.8
1486.0	11.1
1496.7	8.3
1499.6	3.7
1502.0	5.2
1506.0	4.4
1516.5	9.9
3055.9	6.4
3059.9	25.8
3063.4	20.1
3066.8	24.7
3107.1	15.8
3112.8	8.0
3123.6	13.2
3129.8	28.5
3131.6	0.4
3142.3	28.8
3154.1	7.4
3157.0	15.6
3186.7	7.3
3876.0	35.1

Table S149: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol ((H-bonded)

Frequency	IR Intensity
131.4	1.7
159.7	0.3
213.5	0.3
232.9	0.1
241.4	1.2
260.4	0.2
282.3	0.1
323.8	1.5
342.8	0.5
357.4	0.5
414.9	25.1
415.6	51.0
456.8	21.2
496.2	11.6
576.2	8.3
613.5	0.4
635.7	3.2
674.5	14.2
757.5	0.4
797.0	4.0
835.8	2.1
914.7	0.7
935.4	17.0
962.8	5.0
988.4	1.5
1008.4	8.6
1036.5	9.6
1063.5	10.5
1073.3	33.2
1084.1	8.9
1113.6	12.7
1147.8	17.4
1172.0	9.2
1201.1	31.9
1229.0	18.0
1241.9	5.2
1257.8	6.1
1313.0	2.2
1327.1	0.4
1333.2	1.1
1372.7	44.8
1394.7	28.3
1400.2	11.3
1416.8	3.5
1420.0	6.0
1482.6	0.8
1487.6	14.6
1493.7	9.4
1499.4	4.9
1506.2	8.2
1507.7	6.3
1521.6	4.2
3062.1	5.6
3064.7	18.6
3074.8	16.0
3078.9	28.4
3097.2	14.0
3108.8	1.9
3123.5	14.4
3128.0	26.6
3133.2	14.2
3139.3	30.3
3143.3	12.1
3152.5	6.7
3186.2	5.4
3822.8	25.9

Table S150: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of trans-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol

Frequency	IR Intensity
92.5	0.0
114.5	0.9
173.8	1.1
210.9	0.3
235.8	1.9
243.5	13.2
282.2	52.5
294.5	16.6
302.6	24.8
330.5	0.6
348.6	2.7
415.8	5.0
422.5	1.1
484.9	1.9
575.2	6.6
619.9	4.2
653.3	2.8
678.0	25.8
778.1	8.7
795.9	1.1
842.4	0.7
914.2	2.5
950.9	16.5
973.4	4.7
983.5	21.1
1000.4	30.7
1018.5	7.2
1035.5	2.2
1064.8	6.4
1081.5	25.5
1103.2	2.1
1146.2	1.3
1189.1	29.4
1202.2	6.1
1227.5	0.8
1236.3	18.7
1257.5	14.4
1317.0	6.3
1322.7	6.6
1342.8	3.1
1353.2	6.0
1387.1	8.6
1401.6	15.0
1413.6	4.3
1422.9	2.9
1478.3	3.7
1483.5	6.2
1488.1	3.0
1492.4	6.7
1502.6	7.6
1505.1	7.7
1514.7	5.9
3057.8	14.7
3066.2	13.1
3070.6	22.9
3074.5	21.8
3090.9	20.1
3104.6	1.4
3126.8	27.1
3127.3	11.4
3137.4	17.4
3139.4	15.6
3141.9	14.0
3155.3	6.0
3193.9	5.8
3873.4	33.0

Table S151: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-thiirane-1-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
83.1	0.3
112.4	0.3
186.2	1.6
208.6	1.6
228.0	78.7
234.4	11.7
281.5	4.8
295.5	0.8
335.0	1.4
357.4	1.0
368.8	1.5
387.7	1.1
445.8	4.5
505.8	11.6
567.9	2.9
624.1	4.0
635.9	1.2
714.4	14.7
754.1	1.7
808.9	4.3
840.0	10.9
912.5	7.2
945.0	2.5
951.6	0.9
968.1	5.7
996.0	5.2
1016.5	2.3
1030.9	4.3
1067.9	1.7
1084.2	9.9
1109.4	32.7
1144.4	20.0
1184.6	35.9
1206.8	7.7
1211.4	8.3
1236.8	48.0
1263.1	2.7
1312.7	4.8
1323.8	3.0
1332.5	20.4
1362.1	2.4
1382.1	2.5
1396.9	21.3
1405.9	6.1
1411.8	8.9
1482.6	2.8
1488.4	1.7
1495.5	7.5
1498.8	10.8
1505.8	3.9
1509.7	3.6
1514.7	9.3
3055.3	10.9
3057.2	26.5
3071.3	19.2
3075.8	13.1
3092.5	23.8
3121.2	17.6
3122.7	12.2
3124.0	17.8
3133.6	21.1
3150.4	9.9
3152.3	11.9
3158.1	17.7
3191.1	6.1
3870.3	36.5

Table S152: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of cis-2-ethyl-2,3-thiirane-1-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
89.4	0.6
110.6	1.5
182.7	0.5
206.5	0.2
235.0	0.8
275.4	0.1
291.6	0.4
330.1	0.2
351.9	2.8
368.3	0.7
384.2	3.9
422.3	65.3
446.7	23.6
506.4	17.9
568.6	6.0
616.8	3.2
639.1	2.2
707.1	13.6
754.8	1.0
808.1	3.3
835.4	7.2
916.1	2.0
946.2	3.8
958.1	1.0
972.3	4.5
996.6	11.6
1021.4	16.3
1032.0	16.6
1068.8	7.9
1086.3	7.6
1107.4	8.6
1150.8	20.7
1169.0	8.5
1210.5	2.9
1233.0	27.0
1246.7	55.4
1252.4	1.6
1322.9	10.2
1323.0	2.2
1348.7	2.7
1363.2	1.7
1382.1	53.0
1398.9	6.1
1411.8	8.6
1419.4	24.5
1482.7	3.0
1485.5	5.9
1492.6	4.3
1499.3	13.1
1505.3	4.3
1510.5	3.4
1515.5	4.3
3058.0	20.1
3068.4	6.8
3071.3	18.3
3074.8	17.3
3101.5	12.3
3120.5	2.8
3125.0	18.2
3133.9	21.4
3144.3	15.8
3147.4	14.5
3153.0	17.5
3163.1	13.0
3191.5	4.9
3823.6	25.6

Table S153: M06-2X/aug-cc-pVTZ Frequencies and IR Intensities of trans-2-ethyl-2,3-thiirane-1-methylcyclopentan-1-ol

Frequency	IR Intensity
49.7	0.1
115.5	1.2
200.7	0.7
209.8	5.6
228.3	1.0
242.8	86.1
253.7	4.9
275.4	3.0
310.9	1.2
330.3	1.6
351.8	3.5
403.2	4.3
426.9	0.9
515.5	6.7
571.7	5.3
611.1	2.0
633.4	2.5
673.1	23.9
775.8	2.6
816.1	14.5
841.9	7.6
905.0	11.2
938.8	4.9
958.7	16.2
972.7	1.9
1000.6	4.5
1013.4	2.3
1049.3	6.7
1067.8	0.3
1094.1	33.1
1118.5	5.6
1142.4	2.6
1164.0	50.9
1200.2	1.7
1214.4	5.1
1233.9	13.0
1259.3	21.5
1305.9	4.3
1326.9	4.2
1344.1	7.6
1368.0	8.9
1384.5	7.2
1400.0	1.9
1409.2	16.8
1413.4	15.5
1477.5	3.1
1490.9	5.3
1491.1	2.6
1494.5	3.8
1499.8	4.3
1502.9	9.3
1513.6	5.3
3055.3	15.6
3062.6	15.2
3069.4	23.5
3074.7	21.1
3091.7	26.6
3108.3	2.2
3124.3	13.8
3128.7	14.0
3135.5	23.5
3145.1	4.3
3146.7	12.8
3149.3	17.8
3203.1	5.1
3869.8	36.7

Table S154: M06-2X/cc-pV(T+*d*)Z optimized geometry of cis-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å)

Atom	x	y	z
C	0.979775	−0.011587	0.249791
C	−0.344244	0.592129	−0.228742
C	−1.118624	−0.507834	−0.882176
C	−0.292458	−1.784654	−0.835357
C	0.701741	−1.525972	0.302205
C	−0.320215	1.995624	−0.776308
P	−1.811370	0.014250	0.769493
C	2.104027	0.295014	−0.737060
O	1.298672	0.533988	1.520595
H	3.014538	−0.223817	−0.429446
H	1.849495	−0.041254	−1.743275
H	2.310035	1.363402	−0.766134
H	2.182489	0.246372	1.765361
H	0.247391	−1.752892	1.267350
H	1.614652	−2.114888	0.214124
H	−0.893964	−2.677709	−0.671078
H	0.234782	−1.910201	−1.784223
H	−1.710293	−0.297082	−1.762614
H	0.302448	2.057491	−1.671506
H	−1.322167	2.325449	−1.045174
H	0.078597	2.686339	−0.032604
H	−2.687220	0.974611	0.216344

Table S155: M06-2X/cc-pV(T+*d*)Z optimized geometry of cis-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å)

Atom	x	y	z
C	0.969279	0.000150	0.241770
C	−0.343062	0.600348	−0.292568
C	−1.108438	−0.501780	−0.936837
C	−0.288338	−1.781503	−0.857733
C	0.687094	−1.515378	0.293109
C	−0.306929	1.997515	−0.853558
P	−1.836875	0.037180	0.695807
C	2.127934	0.300572	−0.698224
O	1.350736	0.535222	1.494636
H	3.022697	−0.198532	−0.328603
H	1.914570	−0.056095	−1.706621
H	2.323810	1.370369	−0.734528
H	0.589608	0.479398	2.082418
H	0.217938	−1.752792	1.249921
H	1.603982	−2.098010	0.226958
H	−0.897458	−2.670072	−0.698464
H	0.254410	−1.914937	−1.796445
H	−1.696734	−0.304872	−1.822942
H	0.332603	2.042303	−1.737439
H	−1.301970	2.330783	−1.143368
H	0.086925	2.695314	−0.113670
H	−2.697761	1.005992	0.138552

Table S156: M06-2X/cc-pV(T+*d*)Z optimized geometry of trans-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (in Å)

Atom	x	y	z
C	−0.302990	0.610814	−0.270024
C	1.028066	−0.009118	0.168894
C	0.700641	−1.498127	0.357235
C	−0.346615	−1.796074	−0.722295
C	−1.139298	−0.502731	−0.811949
C	1.658029	0.642343	1.385942
O	1.883820	0.143976	−0.968272
P	−1.741764	0.152677	0.828464
C	−0.250853	1.967132	−0.923677
H	−1.767481	−0.328359	−1.674559
H	0.146898	−1.971635	−1.679477
H	−0.960641	−2.663943	−0.486766
H	1.598680	−2.109434	0.267031
H	0.286089	−1.665387	1.352992
H	−1.232716	2.246220	−1.303869
H	0.064339	2.735597	−0.216531
H	0.456768	1.953149	−1.752104
H	2.595617	0.143142	1.641894
H	1.874819	1.690741	1.181901
H	0.992519	0.579695	2.246163
H	2.745234	−0.219119	−0.744695
H	−2.604866	1.114993	0.260464

Table S157: M06-2X/cc-pV(T+*d*)Z optimized geometry of cis-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å)

Atom	x	y	z
C	0.406096	−1.476311	0.330879
C	0.638708	0.047548	0.290858
C	−0.681073	0.600001	−0.266006
C	−1.378307	−0.527573	−0.957987
C	−0.509277	−1.771234	−0.862229
C	1.802652	0.422561	−0.639884
C	3.169609	−0.069087	−0.175407
O	0.853189	0.603430	1.579271
C	−0.695626	2.003213	−0.817623
P	−2.177546	−0.034174	0.653371
H	3.219904	−1.154529	−0.096958
H	3.941708	0.241834	−0.877933
H	3.436461	0.357083	0.793026
H	1.588897	0.038711	−1.641230
H	1.835251	1.509281	−0.714772
H	1.649951	0.217614	1.952476
H	−0.101680	−1.712428	1.266949
H	1.331198	−2.048991	0.305374
H	−1.083851	−2.687300	−0.730972
H	0.077092	−1.876188	−1.778410
H	−1.927275	−0.338535	−1.870500
H	−0.053226	2.089927	−1.696212
H	−1.702517	2.290121	−1.115415
H	−0.347882	2.712290	−0.065550
H	−3.059686	0.892142	0.054489

Table S158: M06-2X/cc-pV(T+*d*)Z optimized geometry of cis-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å)

Atom	x	y	z
C	−0.365120	1.473067	0.739010
C	−0.568626	−0.058120	0.673671
C	0.482370	−0.527642	−0.348313
C	0.963024	0.661785	−1.101848
C	0.215769	1.896018	−0.617819
O	−0.406049	−0.681235	1.936312
C	−1.990712	−0.439202	0.256430
C	−2.487338	0.186013	−1.040727
C	0.306332	−1.882234	−0.983744
P	2.215677	0.029768	0.126197
H	−1.290048	1.991496	0.989061
H	0.347371	1.686474	1.537546
H	−0.577023	2.133002	−1.327713
H	0.859463	2.771132	−0.537970
H	1.214183	0.574313	−2.150606
H	1.136541	−2.113606	−1.649061
H	0.255202	−2.657110	−0.217979
H	−0.614666	−1.924616	−1.568792
H	0.523835	−0.617243	2.179294
H	−1.802130	0.005265	−1.870885
H	−3.456430	−0.229531	−1.313415
H	−2.611959	1.264156	−0.941382
H	−2.040605	−1.527233	0.200865
H	−2.640999	−0.144962	1.082227
H	2.856304	−0.852755	−0.768727

Table S159: M06-2X/cc-pV(T+*d*)Z optimized geometry of trans-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (in Å)

Atom	x	y	z
P	1.645617	0.077802	−1.760429
C	0.886522	0.630762	−0.146117
C	−0.472890	−0.013671	0.149818
C	−0.222878	−1.517543	−0.053412
C	1.224657	−1.729261	0.407529
C	1.918560	−0.437751	0.011683
C	−1.616070	0.552739	−0.685099
C	−2.971428	−0.070902	−0.371385
O	−0.690867	0.243356	1.540668
C	1.109225	2.034919	0.353339
H	−0.937307	−2.120627	0.506699
H	−0.334081	−1.773548	−1.109158
H	1.256714	−1.825343	1.494028
H	1.679513	−2.617042	−0.029285
H	2.874230	−0.195769	0.455913
H	2.147329	2.331050	0.207269
H	0.480101	2.750611	−0.177244
H	0.873009	2.092550	1.415536
H	−2.963247	−1.148595	−0.539702
H	−3.268681	0.112357	0.662812
H	−3.749304	0.354924	−1.003363
H	−1.659116	1.630174	−0.512600
H	−1.374880	0.403644	−1.739099
H	−1.479150	−0.233102	1.814110
H	2.639434	1.080812	−1.747539

Table S160: M06-2X/cc-pV(T+*d*)Z optimized geometry of cis-2-ethyl-2,3-phosphirane-methylcyclopentan-1-ol (not H-bonded) (in Å)

Atom	x	y	z
C	−0.318030	1.018488	−0.312413
C	0.328388	−0.368976	−0.199994
C	−0.291355	−1.046060	0.983390
C	−1.277522	−0.088153	1.634898
C	−1.616013	0.895312	0.509219
C	1.798304	−0.508368	−0.563202
C	2.766529	−0.305360	0.602605
P	−0.870876	−1.733135	−0.647708
C	0.570152	2.114314	0.272367
O	−0.555663	1.290926	−1.685435
H	1.518573	2.177121	−0.258641
H	0.060793	3.076466	0.179472
H	0.766195	1.943662	1.331042
H	−0.845861	2.203049	−1.772006
H	−2.391133	0.484345	−0.138436
H	−1.962345	1.861584	0.875841
H	−2.159358	−0.588911	2.032527
H	−0.787439	0.429582	2.463291
H	0.305520	−1.689513	1.614543
H	1.980802	−1.495213	−0.985767
H	2.009414	0.201444	−1.366115
H	2.674263	0.680770	1.052901
H	2.589963	−1.044436	1.384516
H	3.796356	−0.422641	0.264866
H	0.131450	−2.727211	−0.701648

Table S161: M06-2X/cc-pV(T+*d*)Z optimized geometry of cis-2-ethyl-2,3-phosphirane-methylcyclopentan-1-ol (H-bonded) (in Å)

Atom	x	y	z
C	−0.366063	0.999488	−0.268261
C	0.301749	−0.385210	−0.144589
C	−0.292334	−1.059971	1.043612
C	−1.271009	−0.105054	1.712030
C	−1.639666	0.874327	0.593641
C	1.762591	−0.523711	−0.538640
C	2.749451	−0.281200	0.603687
P	−0.909272	−1.763661	−0.568915
C	0.519530	2.117077	0.264463
O	−0.635866	1.353092	−1.611771
H	1.456857	2.170097	−0.286492
H	−0.005985	3.062399	0.133796
H	0.733305	1.976984	1.323886
H	−1.080673	0.607134	−2.028563
H	−2.443273	0.464089	−0.020648
H	−1.972730	1.843615	0.960019
H	−2.138530	−0.610456	2.133968
H	−0.760591	0.415885	2.525724
H	0.311544	−1.710833	1.660817
H	1.946153	−1.519557	−0.939634
H	1.950749	0.170392	−1.361023
H	2.651012	0.714631	1.029961
H	2.596657	−1.003516	1.406018
H	3.773934	−0.393820	0.249004
H	0.092488	−2.751708	−0.666113

Table S162: M06-2X/cc-pV(T+*d*)Z optimized geometry of trans-2-ethyl-2,3-phosphirane-methylcyclopentan-1-ol (in Å)

Atom	x	y	z
C	0.558946	0.793338	0.086529
C	1.843881	0.084814	−0.379904
C	1.387241	−1.286612	−0.894236
C	0.143629	−1.609023	−0.082198
C	−0.392582	−0.336691	0.497570
C	−1.887540	−0.045226	0.516528
H	−2.031048	0.974230	0.881222
C	−2.584124	−0.214086	−0.832642
H	−2.495630	−1.240889	−1.189312
H	−3.646991	0.009478	−0.737950
H	−2.153326	0.445141	−1.580553
H	−2.370018	−0.698831	1.245341
H	−0.546373	−2.340389	−0.483064
H	1.095395	−1.209602	−1.943455
H	2.165388	−2.044823	−0.817370
H	2.332862	0.675291	−1.154694
H	2.550970	−0.013247	0.441594
C	0.798363	1.834955	1.166133
H	1.249535	1.385032	2.049426
H	1.472407	2.613001	0.799025
H	−0.142135	2.305187	1.452592
O	−0.072564	1.414169	−1.039453
H	0.458105	2.173048	−1.297532
P	0.202275	−1.557788	1.773182
H	1.535787	−1.112509	1.892110

Table S163: M06-2X/cc-pV(T+*d*)Z optimized geometry of cis-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å)

Atom	x	y	z
C	−0.266722	0.792094	0.052481
C	−1.576906	0.194750	−0.303485
C	−1.415914	−1.308106	−0.448125
C	−0.117901	−1.613728	0.310113
C	0.748285	−0.350621	0.143420
C	1.569606	−0.424741	−1.142774
H	2.227068	−1.295623	−1.106691
H	0.926747	−0.526808	−2.018802
H	2.184483	0.465740	−1.258990
O	1.602693	−0.106890	1.246033
H	2.292285	−0.776133	1.255505
H	−0.318249	−1.749592	1.370108
H	0.386495	−2.503819	−0.065445
H	−2.270700	−1.862759	−0.065053
H	−1.312906	−1.547161	−1.509781
S	−1.488428	0.816874	1.394809
H	−2.254385	0.727536	−0.957884
C	0.191206	2.127552	−0.469192
H	0.521936	2.048595	−1.506100
H	−0.620811	2.849379	−0.417937
H	1.022586	2.496834	0.131381

Table S164: M06-2X/cc-pV(T+*d*)Z optimized geometry of cis-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å)

Atom	x	y	z
C	−0.010320	−0.026518	−0.019412
C	1.532588	−0.040631	0.038134
C	1.957654	1.431071	0.046348
C	0.860075	2.135989	−0.727500
C	−0.350163	1.289575	−0.741527
C	−1.744167	1.843587	−0.637607
H	−2.468885	1.096113	−0.961192
H	−1.972304	2.118053	0.393469
H	−1.850099	2.725682	−1.265289
S	0.474887	1.439686	−2.363863
H	0.768675	3.212839	−0.671707
H	1.965150	1.828876	1.064448
H	2.946349	1.592546	−0.379397
H	1.891709	−0.590202	0.906115
H	1.913176	−0.537822	−0.852033
O	−0.548701	−1.154328	−0.675549
H	−0.225976	−1.137896	−1.583763
C	−0.608543	−0.032603	1.379574
H	−0.301565	−0.943438	1.891245
H	−0.263385	0.828127	1.954458
H	−1.695672	−0.015663	1.332264

Table S165: M06-2X/cc-pV(T+*d*)Z optimized geometry of trans-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (in Å)

Atom	x	y	z
C	0.721481	−0.397567	0.059524
C	−0.219572	−1.593154	0.276474
C	−1.539854	−1.174283	−0.382035
C	−1.578596	0.328534	−0.191679
C	−0.206428	0.823622	0.067039
S	−1.309381	0.917581	1.506273
H	−2.266058	0.927721	−0.773513
H	−1.510144	−1.376712	−1.454421
H	−2.406168	−1.680806	0.039212
H	0.203703	−2.495979	−0.163922
H	−0.360083	−1.769642	1.340655
C	0.314090	2.117038	−0.496804
H	−0.476337	2.865028	−0.506494
H	1.135289	2.500420	0.109292
H	0.679526	1.957170	−1.510113
C	1.861024	−0.322387	1.056648
H	2.462653	−1.233107	1.013108
H	2.507365	0.525189	0.829642
H	1.474812	−0.216706	2.069671
O	1.228187	−0.424163	−1.278297
H	1.825211	−1.173139	−1.357141

Table S166: M06-2X/cc-pV(T+*d*)Z optimized geometry of cis-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å)

Atom	x	y	z
C	−0.943909	0.593286	−0.035503
C	−1.743757	−0.550953	−0.536162
C	−0.896748	−1.808427	−0.481325
C	0.213880	−1.460475	0.517526
C	0.438815	0.056553	0.357782
C	1.446753	0.368787	−0.760544
C	2.871156	−0.087389	−0.464006
H	2.943890	−1.164616	−0.318427
H	3.532166	0.174796	−1.288912
H	3.263446	0.406831	0.425777
H	1.093882	−0.084981	−1.691205
H	1.456973	1.447763	−0.913152
O	0.838004	0.692447	1.558982
H	1.636936	0.268631	1.882494
H	−0.122142	−1.645463	1.535182
H	1.119751	−2.038605	0.346041
H	−1.465460	−2.689611	−0.189356
H	−0.482160	−1.994122	−1.475613
S	−2.286600	0.076293	1.073067
H	−2.441480	−0.408167	−1.351034
C	−1.059486	1.976398	−0.620391
H	−0.556373	2.037828	−1.586378
H	−2.106877	2.234390	−0.759704
H	−0.609129	2.706701	0.052094

Table S167: M06-2X/cc-pV(T+*d*)Z optimized geometry of cis-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å)

Atom	x	y	z
C	0.404849	0.099056	0.698807
C	−0.697590	0.623333	−0.239583
C	−1.382185	−0.537520	−0.843332
C	−0.719230	−1.820304	−0.381311
C	0.086529	−1.406644	0.857905
H	0.995944	−1.992957	0.982921
H	−0.511737	−1.537074	1.757437
H	−0.065757	−2.175936	−1.179769
H	−1.441639	−2.606802	−0.169772
S	−2.375893	0.314813	0.419720
H	−1.785237	−0.470606	−1.845683
C	−0.499467	1.934257	−0.949723
H	−1.391974	2.198916	−1.512688
H	−0.300107	2.723005	−0.223946
H	0.346336	1.882214	−1.637045
O	0.411793	0.786051	1.933889
H	−0.478918	0.727459	2.298017
C	1.797618	0.341527	0.115801
C	2.085539	−0.372995	−1.198763
H	1.336618	−0.148845	−1.960694
H	3.055270	−0.069573	−1.590342
H	2.111161	−1.454643	−1.067184
H	1.932324	1.418259	0.005431
H	2.509554	0.019057	0.877419

Table S168: M06-2X/cc-pV(T+*d*)Z optimized geometry of trans-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (in Å)

Atom	x	y	z
C	−0.466326	−0.007663	0.136508
C	0.891221	0.651069	−0.140731
C	1.919980	−0.410766	−0.051723
C	1.251230	−1.724615	0.294816
C	−0.216163	−1.507758	−0.096367
H	−0.898625	−2.114177	0.498912
H	−0.375529	−1.753958	−1.144598
H	1.338072	−1.871987	1.373119
H	1.702555	−2.579687	−0.204968
S	1.632257	0.203120	−1.737294
H	2.896764	−0.180781	0.352316
C	1.121894	2.049010	0.364484
H	2.154536	2.343412	0.187053
H	0.474695	2.759722	−0.149596
H	0.906161	2.095384	1.430963
C	−1.606395	0.574038	−0.689188
C	−2.954633	−0.078412	−0.405304
H	−2.930841	−1.148619	−0.614060
H	−3.257949	0.061254	0.634092
H	−3.735610	0.361108	−1.023739
H	−1.665385	1.644503	−0.481661
H	−1.351760	0.458318	−1.744061
O	−0.673412	0.232079	1.531690
H	−1.458343	−0.249088	1.806096

Table S169: M06-2X/cc-pV(T+d)Z optimized geometry of cis-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (not H-bonded) (in Å)

Atom	x	y	z
C	−0.384873	−0.296569	0.465760
C	0.072564	−1.584686	−0.114153
C	1.365202	−1.354742	−0.877163
C	1.908147	−0.044504	−0.293506
C	0.657108	0.767029	0.096763
C	0.187804	1.615156	−1.083475
H	0.962973	2.344248	−1.329197
H	0.014277	1.004177	−1.970038
H	−0.724972	2.155884	−0.839021
O	0.855785	1.598776	1.226172
H	1.436804	2.322546	0.977117
H	2.483719	−0.237968	0.608207
H	2.537934	0.497721	−0.998615
H	2.064729	−2.183230	−0.780176
H	1.127803	−1.240890	−1.938293
S	0.224949	−1.501414	1.686159
H	−0.646002	−2.302091	−0.487151
C	−1.847308	0.100158	0.566882
C	−2.633448	−0.024014	−0.738502
H	−2.625523	−1.053240	−1.097869
H	−3.673281	0.260003	−0.578143
H	−2.235644	0.608018	−1.529508
H	−2.322029	−0.528303	1.317669
H	−1.890128	1.122554	0.948441

Table S170: M06-2X/cc-pV(T+*d*)Z optimized geometry of cis-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (H-bonded) (in Å)

Atom	x	y	z
C	−1.855796	0.006654	0.574593
C	−0.380385	−0.316943	0.443272
C	0.124071	−1.578037	−0.138974
C	1.377409	−1.292822	−0.944365
C	1.886675	0.036736	−0.380033
C	0.627554	0.797327	0.092577
C	0.104088	1.702095	−1.012556
H	−0.817040	2.196386	−0.708714
H	0.852829	2.467703	−1.211068
H	−0.074172	1.139220	−1.929085
O	0.876244	1.649817	1.190247
H	1.154048	1.093352	1.926873
H	2.534095	−0.140282	0.476320
H	2.448728	0.617823	−1.108731
H	2.112422	−2.093208	−0.880746
H	1.089760	−1.186864	−1.993840
S	0.314938	−1.490450	1.666819
H	−0.566480	−2.340269	−0.474828
H	−2.298069	−0.690771	1.283854
H	−1.944231	1.000722	1.018704
C	−2.637923	−0.070826	−0.737015
H	−2.287960	0.646169	−1.475763
H	−2.561573	−1.067031	−1.173683
H	−3.693418	0.128800	−0.554412

Table S171: M06-2X/cc-pV(T+*d*)Z optimized geometry of trans-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (in Å)

Atom	x	y	z
C	0.564779	0.814131	0.063999
C	1.865592	0.103439	−0.348497
C	1.419388	−1.264268	−0.877739
C	0.183499	−1.582779	−0.060675
C	−0.378363	−0.323433	0.484089
C	−1.871183	−0.061727	0.555926
H	−2.028278	0.938902	0.963731
C	−2.593698	−0.195088	−0.784286
H	−2.467466	−1.198403	−1.192690
H	−3.662191	−0.026387	−0.650402
H	−2.214622	0.518971	−1.509322
H	−2.303420	−0.762216	1.269282
S	0.356500	−1.419239	1.738629
H	−0.478885	−2.376395	−0.379010
H	1.118369	−1.187960	−1.924753
H	2.193199	−2.025476	−0.797602
H	2.396723	0.691776	−1.096602
H	2.516766	−0.014449	0.514819
C	0.766975	1.879607	1.124765
H	1.181942	1.443006	2.031797
H	1.461836	2.641272	0.763068
H	−0.178839	2.366332	1.361885
O	−0.059034	1.384377	−1.090063
H	0.470661	2.134265	−1.374830

Table S172: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
119.2	0.0
209.0	2.2
213.8	1.1
236.7	7.2
260.5	80.9
277.1	1.4
309.0	0.9
324.4	7.0
354.2	0.0
383.1	0.8
429.4	3.8
482.1	10.0
560.3	1.4
596.8	0.2
608.6	0.8
653.2	1.3
717.2	1.6
766.6	1.8
838.1	4.2
895.6	8.1
921.9	9.3
945.4	8.7
957.6	1.0
979.0	0.3
989.4	7.0
1015.0	8.2
1053.4	4.3
1087.0	19.3
1105.5	25.1
1141.4	21.8
1177.0	32.9
1204.1	7.9
1235.4	49.6
1238.1	10.2
1262.7	4.3
1323.8	18.6
1330.3	15.7
1367.5	2.2
1396.1	26.4
1403.5	9.3
1412.8	4.5
1488.3	2.4
1489.8	2.8
1496.6	9.0
1499.5	12.1
1510.1	4.7
1516.4	1.6
2430.1	75.8
3053.5	14.5
3055.3	28.4
3059.6	34.4
3081.4	12.9
3114.9	19.5
3117.7	14.4
3122.7	21.6
3129.1	26.5
3143.4	11.9
3151.9	12.7
3196.1	5.4
3870.9	30.5

Table S173: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
126.0	1.7
209.0	0.5
217.2	0.2
236.4	0.2
266.4	1.2
308.4	0.3
316.8	0.6
347.3	11.1
365.9	55.7
386.7	17.8
428.7	5.9
479.3	12.0
560.7	3.1
596.2	0.2
609.1	5.9
643.6	1.5
712.3	1.9
760.6	1.2
833.8	0.4
886.7	8.2
925.8	1.6
949.0	1.8
963.3	4.1
979.6	0.0
990.2	6.4
1016.6	44.6
1052.1	3.7
1090.0	7.8
1101.1	9.8
1142.9	29.6
1168.2	6.4
1210.4	4.4
1238.5	68.7
1245.1	16.7
1263.5	4.8
1324.6	2.9
1340.4	7.9
1379.5	41.7
1383.3	22.4
1414.2	4.3
1418.5	32.9
1482.8	2.2
1490.1	1.7
1494.7	9.0
1498.1	14.3
1509.1	6.1
1517.3	1.0
2442.6	65.3
3055.7	24.8
3062.3	20.7
3069.8	19.1
3077.7	10.7
3118.9	22.3
3119.4	11.4
3135.1	19.1
3142.7	10.8
3144.5	20.5
3157.1	13.2
3195.1	4.6
3837.9	19.5

Table S174: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of trans-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol

Frequency	IR Intensity
119.6	0.7
196.2	0.1
218.4	3.1
236.4	21.4
243.2	4.1
256.4	67.3
293.4	2.1
319.4	1.2
330.4	4.4
390.2	6.1
410.9	2.5
457.4	2.2
562.3	2.6
609.9	0.5
611.2	4.1
654.6	12.0
726.0	2.0
785.2	3.3
826.8	6.5
895.0	7.8
911.6	4.9
945.7	0.7
955.7	22.8
981.0	12.6
988.2	2.2
1019.9	6.1
1056.3	3.8
1081.6	62.6
1096.7	0.3
1140.4	2.1
1179.2	30.4
1207.0	5.2
1227.1	0.5
1238.7	15.2
1258.6	34.0
1323.1	4.7
1342.5	4.1
1366.7	7.7
1395.0	10.7
1408.8	17.8
1412.5	14.3
1484.3	1.2
1486.1	9.2
1493.4	1.7
1498.9	4.2
1499.8	6.6
1504.7	8.1
2433.9	69.9
3054.6	18.4
3062.8	26.8
3075.9	24.8
3076.3	16.4
3118.6	15.0
3123.6	23.2
3129.2	19.2
3129.3	16.0
3143.2	8.1
3148.0	14.2
3199.4	4.4
3871.1	30.1

Table S175: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
65.7	0.1
120.6	0.0
179.1	0.6
211.6	62.4
219.6	1.0
229.2	14.1
277.7	11.1
290.8	10.4
316.4	2.4
342.1	5.8
352.1	2.8
372.7	0.5
428.6	4.6
507.2	7.3
560.2	1.4
595.6	0.6
636.5	1.5
665.0	1.4
730.0	1.6
745.4	1.0
796.7	1.7
841.7	4.4
904.2	8.2
926.0	11.2
944.4	5.5
961.2	4.8
986.0	7.0
1013.1	14.8
1020.7	2.5
1046.3	17.2
1061.7	8.1
1087.1	8.0
1109.6	15.2
1141.0	19.2
1176.5	14.4
1191.9	9.1
1231.7	46.4
1234.7	8.3
1267.4	3.8
1309.1	12.5
1316.3	20.6
1332.8	0.8
1359.8	9.3
1374.0	0.6
1399.2	20.7
1412.0	4.2
1421.6	6.3
1479.8	2.9
1496.4	9.8
1497.6	6.8
1504.3	5.8
1507.4	5.0
1510.4	3.0
1519.5	12.6
2430.7	76.7
3055.2	24.9
3058.1	17.7
3062.7	18.6
3066.4	31.1
3087.6	10.1
3112.1	12.3
3116.2	15.7
3120.9	12.3
3130.6	15.2
3136.1	29.7
3142.7	15.5
3147.9	29.7
3195.1	5.7
3878.4	29.7

Table S176: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
129.8	0.9
154.5	0.2
220.4	0.1
227.5	0.1
234.1	0.4
257.4	0.4
290.5	0.1
315.2	0.7
329.2	3.2
358.1	6.8
372.9	69.9
415.5	4.2
446.6	11.3
476.7	6.1
564.8	2.7
599.7	2.5
603.4	1.8
652.9	2.2
713.4	1.7
748.9	2.6
798.9	2.7
836.0	0.5
892.6	8.6
929.0	4.7
938.4	8.6
961.5	3.3
984.0	10.1
1009.6	7.3
1038.4	17.2
1057.5	6.3
1075.9	28.7
1088.8	10.0
1111.5	14.8
1143.6	20.2
1173.3	8.5
1195.8	23.0
1223.2	24.7
1241.3	7.2
1251.6	6.1
1308.5	3.3
1324.9	1.0
1330.0	2.3
1371.9	41.2
1387.2	12.2
1396.6	31.4
1414.2	12.3
1419.2	2.8
1485.8	0.3
1492.2	9.4
1495.3	14.6
1503.0	2.9
1507.5	15.9
1512.3	2.5
1524.6	3.5
2442.3	63.6
3056.4	22.1
3063.5	12.3
3075.3	14.9
3078.9	14.6
3082.5	33.2
3109.4	1.9
3118.3	18.9
3119.6	14.2
3128.9	24.5
3133.2	37.6
3139.8	18.6
3141.0	13.2
3192.3	4.1
3836.4	20.1

Table S177: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of trans-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol

Frequency	IR Intensity
86.3	0.0
113.7	0.5
174.0	1.2
202.0	0.1
231.4	6.2
240.4	15.9
273.5	41.0
295.3	14.6
303.3	32.4
320.1	0.3
342.0	3.5
410.7	4.5
417.9	1.9
468.3	1.3
556.6	3.0
604.5	3.8
635.7	2.5
655.2	8.6
725.2	2.3
776.3	4.1
794.4	2.2
841.2	5.4
893.4	7.0
929.3	4.8
949.9	4.4
978.2	5.2
978.7	18.8
998.7	49.1
1017.4	4.7
1037.9	2.0
1061.0	2.8
1089.0	27.8
1101.9	0.3
1143.6	1.7
1181.3	23.6
1198.6	2.9
1227.6	0.7
1238.1	20.4
1252.4	24.3
1314.2	12.1
1317.6	2.1
1343.3	3.8
1350.0	6.0
1374.0	4.0
1400.4	16.6
1411.8	6.8
1419.9	5.9
1483.5	2.2
1486.1	6.5
1488.7	3.0
1499.1	5.5
1505.5	12.2
1505.9	5.3
1515.5	5.5
2434.4	71.8
3058.6	13.9
3062.9	18.8
3067.2	28.5
3073.7	9.1
3075.3	28.4
3103.7	2.1
3118.1	19.2
3127.7	41.6
3128.0	11.2
3130.2	15.3
3137.9	23.5
3142.3	9.2
3198.6	4.7
3877.0	27.9

Table S178: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
83.9	0.1
112.1	0.0
186.9	1.0
209.0	1.3
232.4	1.9
250.9	80.5
287.5	12.0
295.7	1.0
317.3	0.5
353.7	0.9
364.9	2.8
386.7	0.3
446.2	3.3
492.1	7.8
558.8	1.6
600.2	0.4
622.0	0.9
692.2	1.4
725.8	1.5
754.0	4.8
804.4	2.6
841.8	5.2
910.1	12.6
920.7	15.8
950.8	0.6
959.4	0.8
967.0	5.1
995.1	0.9
1016.4	7.5
1023.8	1.7
1065.6	1.9
1084.5	8.1
1109.7	25.9
1141.9	24.7
1175.3	30.8
1204.0	2.0
1210.1	25.1
1235.5	40.4
1257.9	6.3
1314.0	1.3
1320.0	16.5
1329.1	20.3
1359.0	1.4
1373.9	6.3
1393.7	21.5
1407.1	11.5
1412.1	8.2
1486.5	1.2
1492.9	1.6
1497.8	5.5
1506.3	14.7
1508.6	3.5
1512.1	1.3
1514.8	9.6
2426.0	74.6
3054.3	14.9
3058.6	33.5
3069.7	22.5
3073.7	14.9
3081.0	13.3
3112.2	5.7
3113.7	20.3
3122.7	27.1
3128.6	26.2
3131.1	25.9
3153.4	12.6
3157.5	20.2
3200.2	4.8
3871.5	30.3

Table S179: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
95.8	0.6
116.7	0.8
194.0	0.2
209.0	0.6
229.7	0.2
279.5	0.5
291.5	0.4
313.7	0.2
344.0	4.5
360.9	1.2
378.7	46.2
392.4	36.1
443.5	3.6
488.2	11.2
559.9	3.0
598.7	0.7
620.7	5.1
684.0	2.1
717.0	1.9
750.8	2.6
802.6	3.1
836.3	0.8
904.7	11.6
925.7	3.9
953.5	0.0
960.7	1.0
972.6	4.3
995.8	2.8
1017.9	33.6
1024.9	11.8
1064.9	2.6
1087.0	3.7
1105.7	11.8
1146.8	21.0
1168.4	9.0
1204.2	1.1
1227.7	34.9
1240.0	43.1
1248.3	15.7
1315.6	3.7
1324.9	12.6
1342.0	2.2
1361.2	2.8
1379.8	11.8
1384.4	50.0
1411.6	8.4
1419.2	34.4
1484.4	2.6
1489.9	4.5
1495.5	6.0
1505.0	14.2
1508.1	4.4
1510.4	0.9
1516.4	4.3
2444.2	63.4
3061.6	23.4
3068.8	10.8
3071.2	19.8
3072.1	21.8
3079.1	9.9
3110.2	6.0
3118.8	22.6
3131.8	23.8
3134.5	20.1
3145.4	24.4
3155.3	14.8
3160.9	14.1
3197.1	4.1
3836.3	20.0

Table S180: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of trans-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol

Frequency	IR Intensity
79.2	0.1
105.9	0.3
189.7	0.5
207.4	0.1
227.8	1.2
247.3	5.9
269.0	72.3
277.2	9.7
291.8	5.0
324.6	0.8
366.6	9.1
406.5	2.1
415.8	4.9
475.6	3.3
565.0	3.3
591.3	1.5
622.5	3.2
678.7	9.0
728.0	2.3
762.6	2.3
815.8	14.2
843.5	3.5
909.0	4.0
915.2	11.1
948.9	3.4
963.9	14.3
970.5	5.3
1005.3	5.9
1018.8	2.1
1045.7	4.1
1070.6	1.7
1095.8	30.4
1101.7	20.9
1137.8	3.4
1178.2	26.6
1206.1	5.1
1212.9	11.9
1234.7	10.5
1251.9	28.2
1316.7	6.3
1321.8	12.2
1338.4	4.0
1362.4	2.0
1374.3	3.8
1390.4	9.9
1409.1	1.8
1413.5	34.9
1483.9	2.8
1487.2	3.0
1494.4	2.7
1496.7	1.5
1500.5	6.4
1501.8	10.4
1514.6	3.8
2455.5	58.3
3053.0	18.1
3062.7	18.9
3069.1	33.6
3069.5	23.6
3092.4	20.2
3097.0	15.5
3116.6	15.2
3122.8	15.6
3127.6	32.1
3136.0	17.1
3149.4	17.1
3178.8	6.1
3182.6	7.2
3867.7	28.2

Table S181: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2,3-thiirane-1,2-dimethylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
123.1	0.2
210.1	35.4
216.5	11.5
223.4	41.9
242.6	9.4
277.4	0.8
329.1	2.0
333.3	1.0
358.5	0.3
383.6	0.9
434.9	6.4
498.1	11.7
573.5	3.1
620.9	0.9
629.9	2.3
679.4	14.2
775.6	0.8
836.4	6.0
914.5	2.6
943.4	4.7
950.0	2.4
985.3	0.9
990.6	8.1
1017.9	7.1
1060.0	1.7
1080.1	19.0
1103.0	34.4
1144.4	18.1
1188.8	36.9
1207.3	9.4
1238.0	1.7
1240.6	59.1
1269.0	2.1
1327.3	4.7
1333.6	22.4
1378.7	0.5
1398.7	33.1
1405.6	1.5
1414.8	6.5
1483.7	2.0
1489.3	11.8
1491.7	5.9
1498.7	11.0
1503.1	2.0
1514.5	1.1
3055.8	10.3
3061.6	25.3
3063.5	23.5
3094.6	22.6
3121.8	20.2
3124.4	18.2
3130.0	11.7
3150.8	9.7
3153.2	11.7
3156.5	8.7
3187.4	7.8
3874.2	34.1

Table S182: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2,3-thiirane-1,2-dimethylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
122.4	2.6
217.5	0.6
228.3	0.2
233.2	0.2
272.8	0.8
324.3	0.6
327.1	0.6
353.1	1.2
379.1	2.8
416.3	62.3
437.1	30.9
502.3	19.0
572.8	6.6
614.4	0.4
630.6	5.4
674.0	10.9
769.0	1.0
832.6	3.0
914.0	0.2
946.8	3.1
959.3	1.5
986.7	8.4
992.2	4.0
1020.8	32.5
1059.1	9.3
1083.0	13.3
1103.6	6.7
1147.3	29.8
1169.6	8.1
1218.3	6.8
1243.0	38.4
1253.2	40.8
1272.7	1.2
1326.3	1.3
1346.5	8.1
1381.7	56.1
1397.8	15.1
1416.5	7.6
1421.4	22.1
1482.3	4.2
1485.4	3.5
1491.1	13.0
1497.0	8.5
1501.7	4.6
1516.0	0.4
3062.6	21.1
3063.2	12.2
3068.5	17.6
3101.6	11.8
3125.3	17.0
3130.0	9.4
3143.7	13.0
3146.9	15.7
3155.1	11.1
3158.0	11.3
3187.7	6.1
3830.8	23.2

Table S183: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of trans-2,3-thiirane-1,2-dimethylcyclopentan-1-ol

Frequency	IR Intensity
118.7	1.0
206.8	0.5
223.0	1.8
238.8	8.1
250.7	4.0
262.9	83.4
300.0	4.6
330.9	1.6
341.6	2.4
392.1	4.8
416.8	2.5
468.6	2.3
581.9	8.3
621.9	0.8
632.0	3.9
679.7	27.0
789.9	6.9
832.5	1.1
907.7	4.6
931.0	6.0
956.0	21.0
982.4	5.6
995.9	0.3
1018.7	6.5
1062.0	9.6
1079.2	53.2
1097.2	8.5
1143.4	1.3
1189.9	35.0
1209.6	9.5
1231.6	1.4
1237.5	13.4
1265.0	22.2
1327.8	4.7
1346.1	6.3
1378.8	10.8
1400.9	7.6
1410.0	26.9
1414.9	3.5
1476.9	4.1
1486.4	8.3
1491.1	4.1
1494.6	5.8
1500.1	6.7
1503.1	3.2
3055.6	17.0
3070.3	18.4
3075.5	20.9
3094.1	23.7
3124.7	15.0
3129.9	13.7
3139.1	10.8
3146.3	6.3
3150.7	17.0
3157.3	6.8
3193.4	6.2
3872.8	34.2

Table S184: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol ((not H-bonded)

Frequency	IR Intensity
72.9	0.3
123.7	0.6
180.7	3.6
195.5	79.1
223.0	1.4
229.2	3.0
281.7	19.7
287.6	1.1
329.6	1.6
350.7	1.7
353.1	1.4
369.9	0.7
430.6	7.7
520.8	7.1
571.9	2.8
624.7	3.1
652.7	1.4
681.3	16.1
754.1	1.4
798.0	2.1
837.5	5.5
914.5	2.9
941.6	4.8
961.2	6.2
991.0	8.8
1015.9	9.9
1021.5	5.9
1043.3	16.1
1069.8	8.2
1079.5	10.2
1107.8	16.8
1143.7	16.1
1184.3	13.1
1198.8	17.9
1232.5	14.2
1234.3	43.1
1272.6	1.7
1311.9	3.9
1325.8	17.7
1331.3	0.3
1363.8	7.6
1383.6	0.2
1400.5	21.6
1412.7	2.4
1422.9	9.6
1478.9	3.0
1486.2	11.0
1497.3	8.7
1500.2	3.7
1502.3	4.8
1507.3	4.6
1517.3	9.5
3057.3	6.0
3061.2	25.7
3063.8	21.3
3067.9	24.8
3107.8	16.9
3115.0	7.0
3125.0	13.5
3131.6	21.6
3133.8	7.3
3143.2	30.2
3154.7	7.7
3157.0	16.9
3187.7	8.0
3881.6	33.6

Table S185: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol ((H-bonded)

Frequency	IR Intensity
130.8	1.7
158.4	0.3
213.4	0.3
235.3	0.2
242.1	1.1
259.8	0.2
281.6	0.1
324.4	1.5
343.7	0.5
358.2	0.4
415.6	7.2
418.2	68.9
457.5	24.0
496.9	12.5
577.0	8.1
615.0	0.4
636.2	3.0
675.3	13.6
759.1	0.3
798.3	3.8
836.7	2.1
914.8	0.8
935.6	17.0
962.8	5.4
989.0	1.7
1008.7	8.3
1037.2	9.6
1064.7	9.6
1074.3	33.0
1085.5	8.7
1114.1	12.7
1149.1	17.0
1173.5	10.7
1202.2	30.3
1230.0	18.4
1242.3	6.0
1258.5	6.6
1313.1	2.3
1327.2	0.3
1333.5	1.2
1373.9	44.4
1397.6	36.1
1400.6	10.3
1417.4	5.0
1420.5	5.1
1483.0	1.0
1487.9	14.3
1494.2	9.6
1499.9	4.7
1506.3	9.6
1508.2	5.1
1521.7	4.1
3062.5	6.1
3064.9	19.1
3076.7	15.7
3080.3	29.2
3098.3	14.4
3110.1	1.8
3124.8	14.3
3128.9	25.6
3134.1	16.6
3140.3	32.1
3143.8	11.8
3153.5	7.0
3187.6	5.8
3828.0	23.8

Table S186: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of trans-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol

Frequency	IR Intensity
90.8	0.1
114.5	0.9
174.2	1.1
211.6	0.2
236.2	3.3
244.6	17.9
280.1	51.3
297.7	14.4
303.4	24.6
331.6	0.7
349.4	2.3
416.0	4.6
423.7	1.4
485.4	1.8
575.5	6.5
621.7	4.0
654.7	2.3
678.8	24.9
780.2	8.4
798.2	1.2
844.1	0.8
914.3	2.6
952.3	15.3
974.8	4.7
984.7	20.8
1002.6	30.5
1019.1	6.8
1036.3	2.1
1066.1	5.8
1083.0	25.6
1104.2	2.0
1147.0	1.2
1190.4	28.8
1202.8	7.9
1228.5	0.7
1236.9	18.9
1259.0	15.7
1317.6	5.8
1323.6	7.7
1344.3	3.8
1353.9	6.3
1387.4	9.1
1402.5	14.9
1414.2	5.2
1423.6	3.6
1478.2	3.7
1484.3	6.3
1488.6	3.2
1492.2	6.1
1503.2	7.4
1505.8	8.1
1515.2	6.1
3058.6	14.4
3067.6	11.7
3071.0	25.4
3075.3	21.9
3092.2	20.2
3105.8	1.3
3128.5	27.8
3129.1	12.6
3138.9	14.1
3140.2	19.9
3143.1	14.8
3156.7	6.2
3194.7	6.4
3878.3	31.2

Table S187: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2-ethyl-2,3-thiirane-1-methylcyclopentan-1-ol (not H-bonded)

Frequency	IR Intensity
85.9	0.3
112.0	0.2
186.9	1.5
209.7	2.0
229.3	66.9
235.6	22.5
281.2	5.2
295.2	0.9
336.2	1.3
357.1	1.0
369.8	1.6
388.2	1.0
445.8	5.0
506.3	11.0
568.3	2.6
626.1	3.5
636.1	1.4
715.6	13.9
756.5	1.8
810.2	3.9
841.0	10.5
913.0	7.4
945.5	2.4
951.5	1.1
968.3	5.7
997.1	5.0
1017.2	2.4
1030.9	4.4
1068.1	1.6
1085.1	9.8
1110.3	31.9
1145.3	19.1
1186.3	37.4
1207.4	7.8
1212.1	8.0
1238.5	48.2
1264.0	3.1
1313.9	4.8
1324.3	3.2
1332.8	23.2
1362.2	2.3
1383.8	1.7
1397.9	23.8
1406.4	6.2
1413.4	9.1
1482.9	3.1
1489.0	1.4
1495.9	8.5
1499.1	9.6
1505.9	4.0
1511.0	4.2
1515.2	9.0
3055.7	11.7
3058.3	26.7
3071.5	19.0
3076.6	13.8
3094.2	23.7
3122.0	18.3
3123.8	11.6
3124.6	19.0
3134.4	21.6
3151.4	10.1
3153.4	12.9
3159.9	18.5
3191.3	7.1
3874.3	34.1

Table S188: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of cis-2-ethyl-2,3-thiirane-1-methylcyclopentan-1-ol (H-bonded)

Frequency	IR Intensity
89.7	0.6
110.0	1.4
181.4	0.6
207.0	0.2
235.2	0.8
275.0	0.1
291.5	0.4
331.1	0.2
351.3	2.5
369.2	0.6
384.6	3.7
423.9	64.0
447.0	28.3
507.2	18.4
569.2	5.7
618.8	2.9
638.9	2.2
707.8	12.9
757.1	1.0
809.5	3.0
836.6	6.8
916.1	2.2
946.5	3.9
958.0	1.1
973.2	4.1
997.7	11.3
1022.3	15.9
1031.9	17.3
1069.3	7.9
1087.1	7.7
1108.0	9.0
1151.6	19.7
1170.0	10.2
1211.0	2.5
1233.5	23.8
1248.5	54.3
1253.3	5.6
1323.3	2.9
1323.6	9.9
1349.1	3.0
1363.9	1.9
1384.7	55.8
1398.7	6.2
1413.1	8.4
1421.2	29.0
1482.9	3.3
1485.9	6.1
1493.3	4.3
1499.7	12.6
1505.5	4.5
1511.0	3.5
1516.1	4.0
3059.5	20.4
3069.1	6.7
3071.6	18.6
3075.5	18.1
3102.6	12.6
3121.2	2.9
3126.4	18.7
3134.9	21.8
3145.3	15.0
3147.8	17.1
3154.2	17.4
3164.7	13.7
3192.2	5.6
3828.9	23.6

Table S189: M06-2X/cc-pV(T+d)Z Frequencies and IR Intensities of trans-2-ethyl-2,3-thiirane-1-methylcyclopentan-1-ol

Frequency	IR Intensity
61.1	0.1
111.8	0.8
191.8	0.8
215.2	0.3
228.6	2.6
248.5	4.3
265.7	79.5
273.5	8.1
299.9	3.8
332.3	1.3
371.5	3.9
407.6	5.9
415.8	1.7
483.2	4.4
576.4	7.1
624.0	2.4
635.2	1.5
712.2	23.0
764.1	2.5
816.4	13.6
842.2	5.3
903.7	9.9
934.7	3.3
962.8	16.2
970.3	4.6
997.9	9.9
1014.3	1.8
1040.3	3.9
1067.4	0.3
1096.6	14.5
1099.8	38.8
1143.8	1.8
1186.5	31.1
1205.7	4.2
1214.1	2.2
1234.1	12.5
1259.7	21.8
1316.1	11.8
1325.9	4.8
1345.0	4.0
1362.0	1.0
1386.7	5.1
1397.8	2.2
1409.4	2.1
1412.6	36.0
1476.4	3.2
1484.5	5.0
1490.8	5.3
1495.4	3.5
1499.2	2.1
1501.3	8.9
1516.3	5.0
3055.3	16.5
3069.4	23.6
3071.5	21.3
3074.0	20.1
3094.0	23.2
3116.9	10.0
3124.4	11.9
3128.6	18.4
3130.4	28.7
3146.0	9.0
3153.6	14.6
3178.3	7.0
3195.9	5.5
3869.5	33.2

Table S190: MP2 optimized geometry of cis-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.250901	0.781870	−0.024895
C	−1.547468	0.186649	−0.359618
C	−1.422827	−1.314060	−0.432466
C	−0.124090	−1.582449	0.342633
C	0.757903	−0.345849	0.097982
C	1.555919	−0.478816	−1.192046
H	2.232575	−1.331970	−1.120704
H	0.898297	−0.643499	−2.046037
H	2.149846	0.414706	−1.371885
O	1.621266	−0.045956	1.189916
H	2.275369	−0.751099	1.242531
H	−0.331988	−1.632847	1.408183
H	0.371060	−2.502917	0.034507
H	−2.282290	−1.824498	0.000935
H	−1.341000	−1.621813	−1.476728
O	−1.292999	0.685257	0.969564
H	−2.301678	0.727579	−0.917076
C	0.184639	2.169807	−0.368139
H	0.640758	2.210347	−1.355892
H	−0.674676	2.836057	−0.351039
H	0.912754	2.516872	0.363866

Table S191: MP2 optimized geometry of cis-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.020445	−0.002940	0.021310
C	1.522366	−0.032406	0.012174
C	1.975240	1.433264	0.024066
C	0.851559	2.140495	−0.687775
C	−0.353801	1.314232	−0.661950
C	−1.757745	1.819656	−0.728508
H	−2.408078	1.053012	−1.148763
H	−2.128485	2.077756	0.262190
H	−1.801222	2.703076	−1.361304
O	0.422326	1.444971	−1.882478
H	0.806238	3.220066	−0.754637
H	2.050111	1.823294	1.041081
H	2.939063	1.580723	−0.462007
H	1.914490	−0.609570	0.847203
H	1.850204	−0.508823	−0.909421
O	−0.592472	−1.106943	−0.670991
H	−0.272987	−1.044052	−1.579916
C	−0.579521	−0.047353	1.428922
H	−0.290875	−0.984461	1.901653
H	−0.189562	0.779577	2.022401
H	−1.665925	0.009473	1.413966

Table S192: MP2 optimized geometry of trans-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	0.724709	−0.411326	0.005455
C	−0.228458	−1.587610	0.280719
C	−1.570646	−1.183894	−0.348661
C	−1.566362	0.318299	−0.217065
C	−0.199550	0.800157	−0.015101
O	−1.124149	0.764707	1.066146
H	−2.328335	0.932729	−0.679865
H	−1.604658	−1.442717	−1.407632
H	−2.422662	−1.648393	0.146468
H	0.175099	−2.511972	−0.132194
H	−0.343889	−1.717250	1.354971
C	0.324530	2.141380	−0.418269
H	−0.491807	2.858745	−0.477817
H	1.044317	2.503844	0.317371
H	0.820879	2.072957	−1.384305
C	1.845109	−0.293867	1.021539
H	2.415062	−1.224395	1.073482
H	2.525265	0.511382	0.744558
H	1.435716	−0.089996	2.010890
O	1.240252	−0.481898	−1.322745
H	1.870299	−1.206222	−1.364824

Table S193: MP2 optimized geometry of cis-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.914661	0.589153	−0.104990
C	−1.700862	−0.547520	−0.592209
C	−0.894959	−1.815630	−0.476451
C	0.190837	−1.433005	0.540491
C	0.449945	0.067483	0.313812
C	1.460821	0.317347	−0.809476
C	2.882300	−0.114927	−0.469707
H	2.947760	−1.179262	−0.249443
H	3.552707	0.087819	−1.302866
H	3.263556	0.437843	0.388300
H	1.117543	−0.199830	−1.709024
H	1.463864	1.384121	−1.033600
O	0.831267	0.759048	1.499507
H	1.619806	0.328457	1.845452
H	−0.194050	−1.549925	1.550427
H	1.091837	−2.034794	0.438407
H	−1.495838	−2.662459	−0.146081
H	−0.466949	−2.066547	−1.448986
O	−1.976628	0.030585	0.699472
H	−2.487423	−0.431220	−1.327133
C	−1.109013	2.015227	−0.510782
H	−0.559907	2.252522	−1.420088
H	−2.166917	2.199602	−0.683040
H	−0.763506	2.673810	0.285237

Table S194: MP2 optimized geometry of cis-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.429518	0.099923	0.657952
C	−0.644184	0.601437	−0.294617
C	−1.367963	−0.543167	−0.845787
C	−0.755153	−1.830145	−0.363654
C	0.078743	−1.395220	0.851736
H	0.974238	−1.999713	0.988496
H	−0.515841	−1.482271	1.758516
H	−0.133919	−2.246806	−1.157253
H	−1.510933	−2.572030	−0.106480
O	−1.948436	0.229254	0.230879
H	−1.906545	−0.483813	−1.783478
C	−0.562691	1.960882	−0.907450
H	−1.481883	2.178759	−1.446599
H	−0.427153	2.709175	−0.126910
H	0.276645	2.031305	−1.597962
O	0.376456	0.824494	1.884254
H	−0.539719	0.761274	2.184167
C	1.833786	0.326004	0.120213
C	2.123125	−0.384301	−1.195846
H	1.419647	−0.092311	−1.975411
H	3.124778	−0.142772	−1.546871
H	2.068139	−1.466211	−1.085343
H	1.984165	1.401214	0.014056
H	2.528982	−0.010911	0.890898

Table S195: MP2 optimized geometry of trans-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	−0.467700	−0.013654	0.207084
C	0.882089	0.635251	−0.054516
C	1.900011	−0.415073	−0.026042
C	1.259718	−1.742787	0.269965
C	−0.213775	−1.501402	−0.089762
H	−0.892433	−2.135417	0.479614
H	−0.375724	−1.693606	−1.148551
H	1.376115	−1.958154	1.332803
H	1.699832	−2.561513	−0.298078
O	1.459464	0.150338	−1.285237
H	2.930341	−0.204049	0.229669
C	1.115862	2.072721	0.275979
H	2.162345	2.324245	0.118436
H	0.510697	2.715631	−0.362990
H	0.848624	2.263869	1.313001
C	−1.582771	0.598131	−0.627247
C	−2.930855	−0.088587	−0.441106
H	−2.888132	−1.137278	−0.731524
H	−3.266934	−0.035771	0.595327
H	−3.697691	0.391747	−1.045943
H	−1.669053	1.652584	−0.359827
H	−1.278893	0.548629	−1.674635
O	−0.681333	0.194440	1.609724
H	−1.501407	−0.254792	1.840617

Table S196: MP2 optimized geometry of cis-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.397907	−0.288417	0.369767
C	0.081462	−1.563664	−0.174268
C	1.414953	−1.366858	−0.850458
C	1.912055	−0.051097	−0.234312
C	0.643257	0.771852	0.053123
C	0.232093	1.598109	−1.157121
H	1.017368	2.320548	−1.387504
H	0.086687	0.970259	−2.036384
H	−0.686427	2.145966	−0.956692
O	0.766866	1.609013	1.199246
H	1.394853	2.305901	0.979994
H	2.398338	−0.248361	0.717333
H	2.605597	0.484687	−0.881917
H	2.098519	−2.196650	−0.673066
H	1.266186	−1.278227	−1.928497
O	0.150094	−1.307227	1.241012
H	−0.595361	−2.357145	−0.465133
C	−1.841248	0.068834	0.600540
C	−2.710144	0.014165	−0.654042
H	−2.700905	−0.985808	−1.085756
H	−3.742857	0.263696	−0.414481
H	−2.369860	0.709222	−1.417933
H	−2.225133	−0.634013	1.339416
H	−1.881894	1.059834	1.055493

Table S197: MP2 optimized geometry of cis-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−1.844531	−0.023744	0.599392
C	−0.392164	−0.307668	0.342810
C	0.138149	−1.569574	−0.172890
C	1.428013	−1.321231	−0.910855
C	1.892041	0.027468	−0.346798
C	0.610854	0.797943	0.042421
C	0.145840	1.716281	−1.068713
H	−0.779406	2.218616	−0.793691
H	0.907878	2.474599	−1.241452
H	−0.010521	1.159508	−1.992255
O	0.801758	1.629337	1.182363
H	1.035818	1.033530	1.905539
H	2.479795	−0.134770	0.554062
H	2.500619	0.596946	−1.046574
H	2.158819	−2.115003	−0.759151
H	1.216583	−1.260130	−1.980355
O	0.236015	−1.271013	1.238287
H	−0.503642	−2.408433	−0.411419
H	−2.200140	−0.783909	1.295007
H	−1.924118	0.938112	1.109682
C	−2.708700	−0.038856	−0.659494
H	−2.399106	0.718330	−1.375461
H	−2.652268	−1.008600	−1.152516
H	−3.751768	0.147564	−0.408494

Table S198: MP2 optimized geometry of trans-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	0.556540	0.796479	−0.022995
C	1.887837	0.079471	−0.304794
C	1.502989	−1.318243	−0.809218
C	0.221590	−1.593717	−0.069993
C	−0.379606	−0.334957	0.376426
C	−1.851559	−0.137219	0.596361
H	−2.006602	0.748131	1.216642
C	−2.663545	−0.026050	−0.691512
H	−2.515675	−0.908697	−1.312853
H	−3.725749	0.049898	−0.463222
H	−2.365353	0.843147	−1.268822
H	−2.192550	−0.992071	1.181651
O	0.289791	−1.204921	1.321782
H	−0.377503	−2.473879	−0.266501
H	1.296930	−1.310793	−1.880261
H	2.273680	−2.062004	−0.610494
H	2.476348	0.643835	−1.027760
H	2.460987	−0.000895	0.615882
C	0.673562	1.872024	1.038198
H	0.967069	1.428800	1.988745
H	1.430211	2.606377	0.755476
H	−0.275840	2.390145	1.163350
O	0.005230	1.325403	−1.236437
H	0.571469	2.057991	−1.504133

Table S199: MP2 optimized geometry of cis-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.972861	0.006021	0.223197
C	−0.321019	0.610065	−0.291120
C	−1.097081	−0.475700	−0.930889
C	−0.339685	−1.776638	−0.812112
C	0.646660	−1.493931	0.331719
C	−0.366473	2.045494	−0.716673
N	−1.492967	0.031201	0.407678
C	2.104716	0.250106	−0.766400
O	1.277146	0.607572	1.478750
H	3.007897	−0.259432	−0.426388
H	1.852766	−0.137408	−1.753948
H	2.323640	1.312524	−0.849753
H	2.112595	0.234520	1.780208
H	0.158873	−1.654889	1.289341
H	1.544316	−2.110159	0.279558
H	−0.992719	−2.621834	−0.595352
H	0.184628	−1.984557	−1.746516
H	−1.745004	−0.275550	−1.773686
H	0.332486	2.248800	−1.526582
H	−1.366294	2.304927	−1.065658
H	−0.115616	2.692794	0.123726
H	−2.263641	0.682854	0.280466

Table S200: MP2 optimized geometry of cis-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.294684	−0.753316	−0.059863
C	−0.789268	0.301478	0.115259
C	0.003105	1.621486	0.243700
C	1.312311	1.412524	−0.528184
C	1.558337	−0.069324	−0.391383
C	−0.058147	−2.145530	−0.480574
C	−1.739194	0.329316	−1.064549
N	1.318625	−0.549805	0.999816
O	−1.582729	0.033169	1.265740
H	−0.778947	−2.577523	0.214319
H	−0.495358	−2.161119	−1.477856
H	0.830521	−2.777182	−0.493723
H	2.325007	−0.566319	−0.970759
H	1.193696	1.658365	−1.585035
H	2.129842	2.014527	−0.131969
H	−0.575980	2.469703	−0.117088
H	0.221510	1.784320	1.296690
H	−0.947720	−0.062460	1.988243
H	−2.468388	1.124950	−0.922021
H	−1.193482	0.515763	−1.989688
H	−2.274426	−0.613927	−1.152938
H	1.818429	−1.429042	1.109821

Table S201: MP2 optimized geometry of trans-2,3- aziridine-1,2-dimethylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
N	−1.171495	0.680614	1.115587
C	−1.564277	0.251986	−0.256699
C	−1.474014	−1.242755	−0.424716
C	−0.134207	−1.582452	0.245202
C	0.760921	−0.357474	0.002043
C	−0.216013	0.804593	−0.009893
C	1.865878	−0.207272	1.027894
O	1.291355	−0.381771	−1.331283
C	0.238804	2.156086	−0.464060
H	−2.312125	0.833106	−0.778899
H	−1.447668	−1.480003	−1.488479
H	−2.310502	−1.772271	0.030461
H	0.328686	−2.482235	−0.160498
H	−0.276084	−1.719290	1.314643
H	−0.609864	2.836609	−0.538082
H	0.954047	2.583915	0.240025
H	0.716745	2.086106	−1.438621
H	2.492635	−1.100732	1.053124
H	2.497590	0.645867	0.784251
H	1.434344	−0.063283	2.017293
H	1.915918	−1.114330	−1.370163
H	−1.565159	1.605379	1.273608

Table S202: MP2 optimized geometry of cis-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
N	−2.001035	−0.016196	0.690641
C	−0.913349	0.602392	−0.105393
C	0.442352	0.045768	0.298370
C	0.169340	−1.462795	0.440143
C	−0.894554	−1.782745	−0.621223
C	−1.704215	−0.510210	−0.677458
C	−1.056186	2.035589	−0.519657
C	1.472125	0.343589	−0.796222
C	2.878056	−0.152657	−0.479974
O	0.825420	0.666530	1.523413
H	2.915757	−1.233348	−0.353609
H	3.564389	0.105804	−1.284469
H	3.260633	0.312764	0.427961
H	1.122000	−0.095363	−1.733927
H	1.509772	1.423314	−0.940824
H	1.586179	0.185770	1.865385
H	−0.242857	−1.626960	1.432501
H	1.068760	−2.065535	0.327985
H	−1.496706	−2.650387	−0.351666
H	−0.439258	−1.975201	−1.594389
H	−2.427775	−0.335383	−1.462418
H	−0.460650	2.266893	−1.401092
H	−2.097780	2.255518	−0.755809
H	−0.741021	2.692958	0.290916
H	−2.800983	0.609333	0.631562

Table S203: MP2 optimized geometry of cis-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
N	−1.957282	0.060652	0.736250
C	−0.918788	0.612722	−0.176605
C	0.434059	0.054724	0.251074
C	0.174071	−1.464679	0.371871
C	−0.967878	−1.785435	−0.600771
C	−1.765123	−0.506395	−0.628978
C	−1.050374	2.024604	−0.656640
C	1.513464	0.393822	−0.768083
C	2.899309	−0.112736	−0.387807
O	0.845339	0.631624	1.486789
H	2.943275	−1.199915	−0.362880
H	3.640366	0.228921	−1.108743
H	3.178405	0.259701	0.594738
H	1.209074	−0.009410	−1.737671
H	1.550979	1.479207	−0.869015
H	0.097765	0.493174	2.083955
H	−0.145935	−1.669712	1.391013
H	1.069307	−2.050834	0.180201
H	−1.557410	−2.644265	−0.280059
H	−0.588640	−1.991744	−1.603402
H	−2.551940	−0.350905	−1.355116
H	−0.508137	2.183474	−1.587417
H	−2.098342	2.268349	−0.834192
H	−0.657135	2.715030	0.090280
H	−2.757288	0.687913	0.697029

Table S204: MP2 optimized geometry of trans-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
N	1.473318	0.092099	−1.313359
C	0.888302	0.640430	−0.067143
C	−0.461339	−0.000783	0.206057
C	−0.208108	−1.497866	−0.040126
C	1.257815	−1.730265	0.357300
C	1.914760	−0.419146	0.014839
C	−1.573539	0.584438	−0.651124
C	−2.925588	−0.087851	−0.442776
O	−0.688276	0.245808	1.601715
C	1.124646	2.070117	0.307835
H	−0.900270	−2.113033	0.534523
H	−0.347484	−1.718881	−1.096318
H	1.345810	−1.902558	1.430295
H	1.698306	−2.576926	−0.168638
H	2.919728	−0.190121	0.342553
H	2.176730	2.325996	0.178730
H	0.534866	2.741757	−0.317560
H	0.849456	2.238304	1.346750
H	−2.886504	−1.147019	−0.693325
H	−3.263625	0.005872	0.590136
H	−3.688978	0.372146	−1.067759
H	−1.655759	1.648643	−0.422001
H	−1.265100	0.493955	−1.694062
H	−1.494438	−0.223173	1.842034
H	2.170282	0.760603	−1.633602

Table S205: MP2 optimized geometry of cis-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
N	−0.253206	−1.407695	−1.169627
C	0.388399	−0.333889	−0.365492
C	−0.625927	0.754162	−0.053987
C	−1.885183	−0.034625	0.349430
C	−1.365297	−1.310497	1.028893
C	−0.074455	−1.578585	0.292089
C	1.836573	0.014207	−0.608128
C	2.714577	0.007157	0.641610
C	−0.155932	1.647931	1.085404
O	−0.805421	1.531823	−1.235492
H	−0.927851	2.387481	1.307166
H	0.025213	1.071994	1.992900
H	0.754342	2.178680	0.813233
H	−1.414103	2.246198	−1.017729
H	−2.417011	−0.291789	−0.562528
H	−2.541638	0.550871	0.993325
H	−2.070998	−2.137429	0.949766
H	−1.157526	−1.141760	2.087176
H	0.629600	−2.320123	0.644924
H	2.711215	−0.976879	1.108688
H	3.745378	0.252434	0.387715
H	2.373746	0.726143	1.381889
H	2.249029	−0.698503	−1.325655
H	1.873225	0.988836	−1.098635
H	0.497531	−1.911524	−1.635111

Table S206: MP2 optimized geometry of cis-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
N	0.274593	−1.308842	1.247180
C	−0.408447	−0.333982	0.346174
C	0.605835	0.761053	0.029202
C	1.859525	−0.022320	−0.426119
C	1.356335	−1.356883	−0.990251
C	0.096244	−1.608611	−0.200330
C	−1.865153	−0.021136	0.561403
C	−2.699799	0.003403	−0.717353
C	0.132390	1.722740	−1.040827
O	0.857052	1.553276	1.184914
H	−0.773507	2.238553	−0.728154
H	0.907647	2.468470	−1.210028
H	−0.058170	1.197904	−1.976470
H	1.070256	0.913214	1.877884
H	2.480112	−0.204538	0.448055
H	2.445618	0.549890	−1.143262
H	2.089271	−2.156428	−0.882921
H	1.102178	−1.271149	−2.048461
H	−0.582026	−2.407888	−0.468714
H	−2.284193	−0.773977	1.233840
H	−1.938090	0.933305	1.087540
H	−2.360791	0.770150	−1.408359
H	−2.643379	−0.956536	−1.229330
H	−3.746468	0.199702	−0.487955
H	−0.451994	−1.809368	1.753094

Table S207: MP2 optimized geometry of trans-2,3- aziridine-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
N	0.265768	−1.175693	1.385123
C	0.069565	−1.610822	−0.023814
C	1.329712	−1.450368	−0.834927
C	1.849190	−0.076962	−0.385419
C	0.591589	0.753738	−0.078322
C	−0.411845	−0.280754	0.409126
C	0.839836	1.862212	0.924935
O	0.039533	1.278304	−1.295201
C	−1.868548	0.044601	0.603517
C	−2.671511	0.191448	−0.686810
H	−1.957269	0.952032	1.205959
H	−2.576394	−0.705925	−1.297177
H	−3.727463	0.335975	−0.460335
H	−2.317593	1.032621	−1.272877
H	−2.304869	−0.760716	1.201482
H	−0.628246	−2.414114	−0.219381
H	1.074392	−1.442882	−1.894950
H	2.053488	−2.244964	−0.655480
H	2.454550	0.417735	−1.145357
H	2.445295	−0.181450	0.517767
H	1.148684	1.435682	1.877931
H	1.630315	2.527995	0.573049
H	−0.063115	2.453634	1.070990
H	0.673328	1.922736	−1.629940
H	−0.465521	−1.607059	1.945225

Table S208: MP2 optimized geometry of cis-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.982539	−0.011737	0.246814
C	−0.333205	0.593398	−0.235412
C	−1.103524	−0.503469	−0.895890
C	−0.282096	−1.780567	−0.841585
C	0.691800	−1.520714	0.312110
C	−0.326755	2.002887	−0.762697
P	−1.809559	0.000277	0.777423
C	2.102202	0.276646	−0.747447
O	1.305401	0.549674	1.516398
H	3.012488	−0.237194	−0.432141
H	1.845515	−0.078599	−1.745620
H	2.309800	1.343111	−0.796610
H	2.196212	0.257634	1.740205
H	0.215866	−1.731723	1.270280
H	1.601913	−2.117129	0.247505
H	−0.887524	−2.673004	−0.687224
H	0.260964	−1.903091	−1.781541
H	−1.706829	−0.290071	−1.768662
H	0.310635	2.088136	−1.644541
H	−1.331259	2.312230	−1.046083
H	0.040409	2.692790	−0.003187
H	−2.676909	0.967295	0.217471

Table S209: MP2 optimized geometry of cis-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.972489	−0.000656	0.236688
C	−0.330592	0.599953	−0.302503
C	−1.096741	−0.499302	−0.947578
C	−0.279743	−1.778357	−0.865605
C	0.678936	−1.511539	0.298048
C	−0.313693	2.003427	−0.843163
P	−1.827652	0.021104	0.711697
C	2.130710	0.284445	−0.705125
O	1.360475	0.545878	1.489510
H	3.024438	−0.208974	−0.326302
H	1.918677	−0.090267	−1.706153
H	2.327510	1.352455	−0.760522
H	0.576851	0.505334	2.053420
H	0.191023	−1.735316	1.248472
H	1.593246	−2.100406	0.251590
H	−0.890979	−2.667372	−0.715485
H	0.275294	−1.906436	−1.797545
H	−1.702033	−0.300362	−1.822749
H	0.333797	2.070212	−1.718924
H	−1.312723	2.318869	−1.139138
H	0.056231	2.699646	−0.090627
H	−2.681500	0.998838	0.154166

Table S210: MP2 optimized geometry of trans-2,3- phosphirane-1,2-dimethylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	0.700014	−0.384733	0.076517
C	−0.244832	−1.581730	0.257501
C	−1.554483	−1.155454	−0.418850
C	−1.593962	0.352883	−0.252379
C	−0.213762	0.836416	0.057593
H	−2.220519	0.933047	−0.919089
H	−1.505388	−1.375872	−1.486426
H	−2.425987	−1.663396	−0.007696
H	0.186964	−2.471845	−0.200519
H	−0.392182	−1.801686	1.313077
C	0.318757	2.108193	−0.554297
H	−0.437671	2.891950	−0.521221
H	1.192108	2.468944	−0.010875
H	0.601734	1.934716	−1.590991
C	1.819033	−0.322300	1.097250
H	2.438101	−1.220024	1.039769
H	2.453873	0.541860	0.908003
H	1.416726	−0.250390	2.106433
O	1.246425	−0.414119	−1.255513
H	1.845177	−1.168800	−1.292561
P	−1.428450	1.090629	1.468399
H	−1.206015	−0.135433	2.131106

Table S211: MP2 optimized geometry of cis-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.398618	−1.466133	0.347704
C	0.639086	0.053187	0.293939
C	−0.671813	0.601410	−0.271085
C	−1.354812	−0.525486	−0.975378
C	−0.485786	−1.766021	−0.866365
C	1.797933	0.413074	−0.644565
C	3.161258	−0.096555	−0.189067
O	0.849943	0.629569	1.580404
C	−0.707142	2.011600	−0.798205
P	−2.180846	−0.057228	0.652299
H	3.197024	−1.182165	−0.119532
H	3.933587	0.210866	−0.892107
H	3.438287	0.317556	0.780785
H	1.573008	0.027397	−1.642010
H	1.840963	1.498867	−0.722903
H	1.681726	0.280452	1.918530
H	−0.136801	−1.685952	1.272180
H	1.321456	−2.043134	0.354264
H	−1.060830	−2.683944	−0.748683
H	0.122382	−1.865219	−1.768644
H	−1.911138	−0.336541	−1.884306
H	−0.044665	2.128907	−1.657220
H	−1.713984	2.274976	−1.117509
H	−0.400419	2.716471	−0.025568
H	−3.054265	0.873450	0.042649

Table S212: MP2 optimized geometry of cis-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.358932	1.470869	0.740358
C	−0.573803	−0.056853	0.668962
C	0.465455	−0.524227	−0.356162
C	0.952109	0.663390	−1.105637
C	0.209384	1.897103	−0.619939
O	−0.410169	−0.690965	1.933589
C	−1.995538	−0.432686	0.256084
C	−2.491449	0.189202	−1.042168
C	0.313712	−1.883683	−0.982653
P	2.211175	0.043253	0.150440
H	−1.277396	1.993873	1.004727
H	0.365368	1.671699	1.531259
H	−0.589758	2.130147	−1.323237
H	0.853893	2.772398	−0.544745
H	1.227130	0.576197	−2.149309
H	1.147222	−2.099480	−1.649252
H	0.281692	−2.656659	−0.214920
H	−0.607641	−1.943472	−1.564246
H	0.533951	−0.642214	2.135737
H	−1.819278	−0.015365	−1.875360
H	−3.470498	−0.211561	−1.300214
H	−2.596187	1.269095	−0.953858
H	−2.048410	−1.520308	0.202555
H	−2.643424	−0.134093	1.082180
H	2.845758	−0.848661	−0.742558

Table S213: MP2 optimized geometry of trans-2,3- phosphirane-1-ethyl-2-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
P	1.645722	0.077625	−1.764594
C	0.886648	0.630195	−0.143863
C	−0.473132	−0.013960	0.150446
C	−0.223074	−1.517825	−0.052992
C	1.224531	−1.729506	0.407830
C	1.917667	−0.437432	0.013601
C	−1.615878	0.552796	−0.684750
C	−2.971376	−0.070735	−0.371425
O	−0.691498	0.242910	1.541335
C	1.109133	2.034941	0.353394
H	−0.937376	−2.120884	0.507289
H	−0.334274	−1.773734	−1.108706
H	1.256628	−1.826419	1.494301
H	1.679932	−2.616650	−0.029609
H	2.874634	−0.196084	0.455311
H	2.147308	2.330901	0.207497
H	0.480124	2.749812	−0.178349
H	0.872428	2.093823	1.415459
H	−2.963215	−1.148434	−0.539700
H	−3.269019	0.112598	0.662650
H	−3.748979	0.355119	−1.003715
H	−1.658836	1.630209	−0.512098
H	−1.374355	0.403802	−1.738651
H	−1.480115	−0.233217	1.814408
H	2.641383	1.082697	−1.750097

Table S214: MP2 optimized geometry of cis-2-ethyl-2,3-phosphirane-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.315436	1.019677	−0.308004
C	0.334535	−0.359806	−0.192116
C	−0.284535	−1.037503	0.989188
C	−1.272577	−0.082203	1.637040
C	−1.617733	0.884804	0.500602
C	1.796825	−0.515437	−0.565782
C	2.769252	−0.299771	0.593766
P	−0.890002	−1.727772	−0.653114
C	0.562411	2.114850	0.287525
O	−0.540061	1.291590	−1.689759
H	1.512949	2.183818	−0.237127
H	0.048971	3.074465	0.193735
H	0.751362	1.941947	1.346266
H	−0.812583	2.213573	−1.758885
H	−2.378889	0.453804	−0.150517
H	−1.981714	1.849650	0.853974
H	−2.150531	−0.585140	2.041233
H	−0.781617	0.447448	2.457063
H	0.305770	−1.696738	1.611333
H	1.966671	−1.512418	−0.970268
H	2.007392	0.178415	−1.382304
H	2.687134	0.694727	1.024213
H	2.586369	−1.022408	1.388260
H	3.796751	−0.434045	0.256105
H	0.120394	−2.716439	−0.702316

Table S215: MP2/cc-pVTZ optimized geometry of cis-2-ethyl-2,3-phosphirane-methylcyclopentan-1-ol (H-bonded) (in Å)

Atom	x	y	z
C	−0.361744	1.002098	−0.260897
C	0.309154	−0.373996	−0.134071
C	−0.288789	−1.056208	1.045860
C	−1.265273	−0.103396	1.715763
C	−1.638788	0.865669	0.591246
C	1.761337	−0.532260	−0.538264
C	2.752262	−0.272309	0.596333
P	−0.935636	−1.747571	−0.582201
C	0.513234	2.122597	0.276781
O	−0.623463	1.359077	−1.611750
H	1.451470	2.181967	−0.270257
H	−0.017871	3.064406	0.145061
H	0.722742	1.982914	1.336103
H	−1.038633	0.585676	−2.016361
H	−2.430786	0.439779	−0.027170
H	−1.986297	1.833216	0.949279
H	−2.130188	−0.609483	2.143054
H	−0.751017	0.423917	2.522620
H	0.304882	−1.729395	1.650361
H	1.931608	−1.540156	−0.915408
H	1.949431	0.141296	−1.377243
H	2.667374	0.734994	0.994540
H	2.589551	−0.971091	1.416192
H	3.774409	−0.408547	0.244025
H	0.071058	−2.732682	−0.687620

Table S216: MP2 optimized geometry of trans-2-ethyl-2,3-phosphirane-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	−0.372774	−0.292285	0.235565
C	0.454980	0.993612	0.175382
C	1.690954	0.601361	−0.646705
C	1.164691	−0.416550	−1.662993
C	0.105830	−1.167354	−0.877842
C	0.786884	1.593346	1.527585
O	−0.348822	1.914581	−0.583922
P	0.685039	−1.751872	0.815475
C	−1.835296	−0.209082	0.627606
C	−2.766633	0.147049	−0.530623
H	−1.939825	0.526215	1.427978
H	−2.689044	−0.592828	−1.326868
H	−3.802060	0.158785	−0.190173
H	−2.520569	1.119538	−0.943822
H	−2.147882	−1.164727	1.049200
H	−0.592266	−1.809743	−1.397810
H	0.684186	0.101253	−2.494718
H	1.948121	−1.061599	−2.058638
H	2.143095	1.478829	−1.109132
H	2.439870	0.142633	0.001307
H	1.368757	0.895441	2.126806
H	1.370919	2.507654	1.402095
H	−0.126108	1.845396	2.065131
H	0.136917	2.747528	−0.609286
H	−0.435799	−2.589190	1.015574

Table S217: MP2 optimized geometry of cis-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.257869	0.789219	0.044515
C	−1.566790	0.193540	−0.319015
C	−1.408103	−1.307650	−0.456111
C	−0.120689	−1.607653	0.320751
C	0.749703	−0.352266	0.140472
C	1.557700	−0.438799	−1.151018
H	2.218851	−1.306153	−1.108973
H	0.907238	−0.556894	−2.018292
H	2.167613	0.451395	−1.285921
O	1.613793	−0.097414	1.241118
H	2.305575	−0.767941	1.224480
H	−0.332346	−1.724274	1.380468
H	0.384974	−2.504135	−0.037649
H	−2.268391	−1.859611	−0.080791
H	−1.289850	−1.550723	−1.515152
S	−1.489747	0.805008	1.403082
H	−2.248014	0.732978	−0.964907
C	0.192044	2.133670	−0.454353
H	0.550169	2.067977	−1.482260
H	−0.634536	2.839519	−0.417694
H	0.999144	2.513576	0.170842

Table S218: MP2 optimized geometry of cis-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.010344	−0.025642	−0.014502
C	1.530768	−0.040910	0.028892
C	1.952652	1.430616	0.055867
C	0.856018	2.135709	−0.714181
C	−0.352951	1.286771	−0.729179
C	−1.746873	1.839415	−0.650456
H	−2.465165	1.096945	−0.996614
H	−1.995840	2.106675	0.376946
H	−1.836217	2.725678	−1.274608
S	0.485792	1.421078	−2.365982
H	0.764181	3.213894	−0.674360
H	1.952304	1.817274	1.078182
H	2.942548	1.599927	−0.364679
H	1.895105	−0.602369	0.887175
H	1.903331	−0.522925	−0.872404
O	−0.561347	−1.159055	−0.664414
H	−0.245106	−1.115801	−1.576928
C	−0.594129	−0.028400	1.388454
H	−0.289415	−0.942010	1.895828
H	−0.234109	0.827195	1.959985
H	−1.680722	−0.001019	1.354191

Table S219: MP2 optimized geometry of trans-2,3-thiirane- 1,2-dimethylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	0.721318	−0.399852	0.058642
C	−0.221914	−1.588751	0.286354
C	−1.534269	−1.175207	−0.389512
C	−1.572264	0.325397	−0.204375
C	−0.200017	0.819319	0.058550
S	−1.306162	0.903813	1.516936
H	−2.263678	0.931573	−0.775376
H	−1.490632	−1.380420	−1.460733
H	−2.405211	−1.679890	0.024929
H	0.202345	−2.497769	−0.140267
H	−0.371774	−1.748557	1.351581
C	0.314612	2.119476	−0.489535
H	−0.481360	2.861179	−0.493549
H	1.130555	2.502965	0.122328
H	0.682546	1.970261	−1.503051
C	1.863558	−0.320254	1.049256
H	2.468172	−1.228021	1.004305
H	2.505936	0.528657	0.820334
H	1.478830	−0.215466	2.062274
O	1.218782	−0.429308	−1.290659
H	1.801345	−1.194484	−1.355312

Table S220: MP2 optimized geometry of cis-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.936218	0.593377	−0.040947
C	−1.724656	−0.551754	−0.557649
C	−0.876365	−1.805058	−0.490340
C	0.209075	−1.452173	0.533162
C	0.438223	0.060112	0.361678
C	1.440552	0.358183	−0.762184
C	2.861776	−0.112238	−0.472742
H	2.921898	−1.189496	−0.329474
H	3.520821	0.144510	−1.300280
H	3.265481	0.375242	0.414615
H	1.078900	−0.099535	−1.686722
H	1.458169	1.435707	−0.921511
O	0.832114	0.714615	1.561849
H	1.672373	0.332225	1.836161
H	−0.152781	−1.624485	1.543765
H	1.118773	−2.031600	0.388145
H	−1.448094	−2.689112	−0.212005
H	−0.438801	−1.985070	−1.475733
S	−2.293653	0.054557	1.071062
H	−2.424584	−0.406645	−1.370930
C	−1.067759	1.983238	−0.600250
H	−0.540221	2.076321	−1.549765
H	−2.117519	2.217210	−0.762078
H	−0.655974	2.709765	0.099403

Table S221: MP2 optimized geometry of cis-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	0.409554	0.097174	0.694536
C	−0.683537	0.619880	−0.245079
C	−1.373901	−0.539816	−0.845707
C	−0.715864	−1.821544	−0.382502
C	0.083686	−1.404660	0.858763
H	0.990826	−1.993040	0.991195
H	−0.520609	−1.525799	1.755147
H	−0.058664	−2.176644	−1.177661
H	−1.440328	−2.607028	−0.172483
S	−2.368998	0.307204	0.444989
H	−1.796116	−0.468837	−1.840649
C	−0.505340	1.935765	−0.946514
H	−1.402499	2.187304	−1.508025
H	−0.321031	2.724415	−0.217697
H	0.341098	1.898579	−1.632881
O	0.419243	0.792500	1.933049
H	−0.487324	0.738876	2.266046
C	1.801657	0.335714	0.115305
C	2.087819	−0.374598	−1.201141
H	1.354183	−0.126807	−1.968266
H	3.067935	−0.087721	−1.578509
H	2.090665	−1.456319	−1.078789
H	1.940099	1.411859	0.007764
H	2.511246	0.007590	0.876618

Table S222: MP2 optimized geometry of trans-2,3-thiirane- 1-ethyl-2-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	−0.466783	−0.012036	0.137242
C	0.885233	0.649156	−0.130872
C	1.916274	−0.410691	−0.037344
C	1.248960	−1.723079	0.304701
C	−0.212459	−1.507304	−0.106986
H	−0.900438	−2.119506	0.475651
H	−0.354317	−1.743561	−1.159597
H	1.321139	−1.865245	1.384665
H	1.707465	−2.578768	−0.188032
S	1.621083	0.190069	−1.745742
H	2.897700	−0.175455	0.354002
C	1.119374	2.050672	0.356258
H	2.151437	2.339865	0.168741
H	0.471513	2.756904	−0.161802
H	0.910841	2.107389	1.423217
C	−1.605013	0.574978	−0.682518
C	−2.954232	−0.076348	−0.401659
H	−2.936988	−1.142217	−0.625551
H	−3.251128	0.050562	0.640071
H	−3.735449	0.376050	−1.009631
H	−1.662641	1.643859	−0.469400
H	−1.348606	0.463114	−1.737092
O	−0.665674	0.221026	1.542651
H	−1.458900	−0.263932	1.795789

Table S223: MP2 optimized geometry of cis-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (not H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−0.470766	−0.207793	0.062078
C	−0.002122	−1.382243	−0.715192
C	1.442585	−1.167775	−1.120431
C	1.941160	−0.106606	−0.133469
C	0.707310	0.762167	0.164185
C	0.571995	1.868479	−0.878647
H	1.461640	2.500334	−0.852138
H	0.485654	1.456963	−1.884861
H	−0.296250	2.490850	−0.676075
O	0.711025	1.323463	1.471519
H	1.386024	2.011006	1.486671
H	2.263629	−0.569863	0.795278
H	2.763268	0.485541	−0.535240
H	2.029092	−2.084860	−1.090154
H	1.465462	−0.788889	−2.145495
S	−0.239433	−1.727204	1.064831
H	−0.678784	−1.910046	−1.374961
C	−1.861665	0.373191	−0.039336
C	−2.997997	−0.638601	−0.043571
H	−3.043454	−1.182068	0.896105
H	−3.947801	−0.128530	−0.197632
H	−2.878861	−1.367625	−0.844478
H	−1.988427	1.073767	0.788735
H	−1.906692	0.960964	−0.959362

Table S224: MP2 optimized geometry of cis-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (H-bonded) (in Å) with the TZ basis set

Atom	x	y	z
C	−1.855254	0.001840	0.579612
C	−0.382635	−0.309381	0.431102
C	0.122496	−1.574219	−0.143715
C	1.374140	−1.290855	−0.947729
C	1.884753	0.033175	−0.374131
C	0.625444	0.797874	0.085287
C	0.112664	1.699327	−1.024848
H	−0.808526	2.196818	−0.729817
H	0.865140	2.461794	−1.219942
H	−0.059214	1.134963	−1.940452
O	0.867614	1.660927	1.184752
H	1.121587	1.082764	1.917147
H	2.520201	−0.150050	0.489334
H	2.455551	0.614646	−1.095927
H	2.107175	−2.093840	−0.888146
H	1.085069	−1.176722	−1.995837
S	0.336618	−1.476554	1.676565
H	−0.566521	−2.346469	−0.461358
H	−2.285121	−0.712240	1.280436
H	−1.948406	0.987617	1.039977
C	−2.639457	−0.063683	−0.730880
H	−2.291792	0.661420	−1.461098
H	−2.560796	−1.054803	−1.176396
H	−3.694911	0.130955	−0.544492

Table S225: MP2 optimized geometry of trans-2-ethyl-2,3- thiirane-1-methylcyclopentan-1-ol (in Å) with the TZ basis set

Atom	x	y	z
C	0.565237	0.805988	0.047825
C	1.870570	0.089211	−0.330283
C	1.426106	−1.276524	−0.864926
C	0.185820	−1.587475	−0.056514
C	−0.379447	−0.321996	0.470815
C	−1.870618	−0.084209	0.568258
H	−2.042608	0.877989	1.054656
C	−2.599266	−0.133589	−0.774079
H	−2.430133	−1.090767	−1.266780
H	−3.672378	−0.027565	−0.617669
H	−2.260454	0.654845	−1.437173
H	−2.281713	−0.845821	1.230444
S	0.376222	−1.400016	1.756862
H	−0.473276	−2.392756	−0.354198
H	1.132961	−1.197954	−1.913790
H	2.197098	−2.040084	−0.776613
H	2.418660	0.671296	−1.071217
H	2.501464	−0.029612	0.547370
C	0.744376	1.889524	1.091119
H	1.148077	1.469073	2.010198
H	1.438405	2.650129	0.727875
H	−0.207705	2.372708	1.305548
O	−0.045304	1.349808	−1.135472
H	0.518158	2.076055	−1.426740

Table S226: MP2 Frequencies and IR Intensities of cis-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (not H-bonded) with the TZ basis set

Frequency	IR Intensity
130.9	0.8
193.8	1.5
212.0	0.7
228.6	85.2
242.0	8.7
268.9	1.9
300.7	0.5
356.7	2.4
375.5	2.4
417.2	1.4
471.8	12.8
527.4	13.6
580.8	5.6
654.7	1.6
677.4	4.2
797.2	6.0
833.0	3.2
876.9	21.7
940.3	5.4
943.3	8.7
951.3	1.8
991.2	3.1
1005.2	9.8
1037.7	4.5
1075.0	12.2
1094.7	48.5
1119.4	8.8
1160.9	23.3
1206.4	9.4
1224.5	43.7
1237.6	12.3
1259.4	17.6
1301.7	4.2
1328.9	3.4
1337.7	7.7
1398.3	20.8
1404.4	2.9
1408.1	7.1
1471.0	6.2
1486.6	4.0
1496.9	9.9
1502.9	6.3
1504.2	7.3
1512.9	7.4
1519.6	0.2
3063.6	12.7
3080.0	14.8
3083.2	23.8
3104.5	25.5
3139.4	15.5
3147.8	21.0
3166.7	11.3
3173.8	9.7
3175.8	10.7
3181.1	10.3
3197.0	20.3
3829.8	26.8

Table S227: MP2 Frequencies and IR Intensities of cis-2,3-epoxy-1,2-dimethylcyclopentan-1-ol (H-bonded) with a TZ basis set

Frequency	IR Intensity
112.2	3.3
200.3	0.1
209.6	1.2
232.8	1.3
262.7	0.8
292.0	0.6
349.0	4.3
368.8	2.4
409.8	37.7
430.8	38.0
472.6	30.7
532.3	14.2
587.4	4.7
657.0	1.5
671.5	5.2
790.6	3.8
828.2	3.6
876.5	18.9
937.7	5.0
948.5	4.2
956.6	7.6
990.2	19.4
1005.2	11.3
1040.1	14.2
1072.5	13.8
1109.2	2.9
1120.8	17.4
1163.3	41.4
1179.7	3.4
1215.8	39.3
1244.0	6.2
1292.5	13.3
1311.9	1.2
1331.2	2.0
1344.6	0.7
1386.3	32.5
1406.2	11.0
1423.5	30.6
1473.8	5.1
1487.0	7.6
1495.2	9.8
1500.8	5.6
1503.9	5.3
1511.7	5.0
1521.8	0.0
3075.5	8.0
3078.1	15.7
3083.5	24.0
3109.1	16.3
3139.8	16.3
3164.0	8.6
3168.0	12.5
3168.1	16.4
3177.0	15.5
3180.6	8.2
3198.6	19.5
3800.7	27.3

Table S228: MP2 Frequencies and IR Intensities of trans-2,3-epoxy-1,2-dimethylcyclopentan-1-ol with a TZ basis set

Frequency	IR Intensity
118.4	2.1
190.6	0.3
221.0	5.0
243.2	3.8
258.0	62.6
261.9	1.2
277.7	29.8
347.7	2.1
377.5	6.7
418.9	1.3
470.0	13.3
504.1	1.8
596.4	2.6
648.9	1.4
686.7	2.3
797.4	5.8
838.9	4.9
866.9	8.1
934.2	23.9
943.4	10.6
950.4	10.7
988.0	2.6
1011.9	5.9
1037.1	2.3
1079.6	31.3
1090.8	41.4
1117.1	4.0
1160.3	2.3
1209.1	10.4
1217.2	59.1
1239.9	3.4
1256.9	4.7
1301.3	4.1
1335.7	4.6
1346.8	2.8
1399.0	6.8
1403.0	12.3
1413.3	22.7
1473.2	4.1
1482.5	5.4
1493.4	6.7
1497.1	10.7
1503.6	3.5
1514.7	5.5
1517.8	2.2
3063.5	15.7
3078.9	16.3
3091.9	24.7
3103.9	24.4
3147.0	8.2
3149.6	17.3
3163.8	10.7
3166.9	11.8
3173.2	16.3
3186.6	5.8
3202.6	19.4
3826.3	25.9

Table S229: MP2 Frequencies and IR Intensities of cis-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) with a TZ basis set

Frequency	IR Intensity
80.0	0.2
126.3	0.5
174.5	13.8
193.8	77.4
202.3	2.7
225.3	4.0
269.6	14.6
282.4	0.1
315.3	0.7
354.3	1.3
387.9	2.8
418.6	4.2
474.9	10.2
539.2	11.9
584.0	4.6
656.6	1.5
694.6	3.1
781.1	5.7
792.9	2.3
839.4	4.2
875.4	20.5
942.7	0.9
946.7	14.9
971.5	6.5
999.6	19.1
1022.2	4.3
1035.8	18.3
1043.0	10.6
1081.9	11.8
1100.6	14.1
1119.7	8.1
1159.2	20.6
1191.3	4.8
1226.8	46.1
1234.9	5.7
1249.2	18.8
1297.6	1.4
1317.4	1.3
1329.3	3.5
1339.9	7.0
1359.3	4.3
1397.9	7.4
1406.8	7.3
1417.4	5.1
1472.2	5.1
1483.7	7.1
1487.6	9.3
1500.1	6.2
1505.7	7.2
1514.8	3.3
1517.2	5.6
1527.8	7.0
3073.1	6.9
3076.3	21.2
3080.1	17.9
3083.0	26.9
3115.0	21.6
3130.6	9.5
3139.2	14.4
3160.7	21.2
3165.4	22.8
3169.0	10.7
3177.5	11.7
3180.1	11.5
3196.5	20.9
3837.8	25.8

Table S230: MP2 Frequencies and IR Intensities of cis-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) with the TZ basis set

Frequency	IR Intensity
125.6	1.7
132.0	1.1
196.2	0.4
218.4	0.3
234.8	0.5
250.9	2.8
255.7	0.6
300.0	0.8
367.0	4.8
395.9	4.7
430.8	34.1
450.4	17.6
476.6	53.2
526.0	9.9
608.5	4.8
644.7	0.6
675.7	5.9
784.1	0.8
796.0	3.1
832.1	3.5
873.6	16.3
939.0	1.7
942.8	26.1
968.2	9.3
1004.0	3.4
1016.3	17.5
1049.2	11.5
1065.6	37.4
1080.3	3.6
1112.3	1.9
1128.7	24.9
1155.6	21.1
1182.2	11.0
1195.5	17.4
1243.7	1.6
1272.5	2.8
1289.3	7.0
1322.8	0.9
1329.7	7.0
1340.0	2.6
1372.9	12.2
1405.8	11.2
1407.5	30.9
1418.1	4.8
1473.3	5.2
1486.0	8.7
1497.9	5.2
1499.4	8.2
1504.5	6.6
1515.7	1.0
1517.6	10.2
1526.3	4.9
3074.9	11.7
3076.2	12.0
3083.1	19.9
3090.4	27.4
3106.3	18.0
3130.1	5.1
3140.8	12.6
3159.9	24.1
3162.6	7.2
3163.1	34.1
3166.0	14.9
3178.3	8.4
3194.2	19.3
3791.6	26.8

Table S231: MP2 Frequencies and IR Intensities of trans-2,3-epoxy-1-ethyl-2-methylcyclopentan-1-ol with the TZ basis set

Frequency	IR Intensity
98.5	0.4
119.0	1.9
168.8	1.2
193.5	0.6
237.1	13.5
244.8	6.4
261.8	81.3
267.1	6.5
295.5	1.3
357.6	1.9
398.9	2.6
428.9	3.5
478.4	10.9
513.7	2.1
584.7	1.8
672.3	0.4
688.5	2.8
787.0	6.5
804.2	2.5
838.2	6.8
874.2	9.6
944.1	5.7
959.9	33.8
975.6	10.2
986.7	17.3
1016.2	17.2
1028.3	1.6
1044.8	1.5
1083.3	15.1
1097.7	18.2
1119.6	6.0
1162.5	2.0
1203.6	6.3
1211.6	51.9
1239.4	4.7
1247.8	11.3
1299.1	4.3
1319.7	2.3
1332.5	5.1
1345.7	2.4
1355.8	2.4
1402.6	15.7
1407.3	3.7
1422.5	14.8
1474.5	3.5
1483.0	4.0
1487.7	9.2
1493.7	4.2
1500.2	5.5
1516.0	2.2
1516.6	7.9
1524.9	7.0
3069.7	16.0
3076.6	7.7
3079.4	26.5
3091.1	26.9
3102.9	21.0
3128.0	3.9
3145.7	8.3
3152.7	27.0
3164.1	13.6
3164.7	16.8
3167.2	22.2
3185.4	5.8
3201.7	20.4
3832.0	23.0

Table S232: MP2 Frequencies and IR Intensities of cis-2-ethyl-2,3- epoxy-1-methylcyclopentan-1-ol (not H-bonded) with the TZ basis set

Frequency	IR Intensity
82.2	0.2
114.0	1.3
184.0	0.4
200.6	2.8
226.0	21.7
234.1	67.1
272.9	2.3
302.2	2.3
317.4	0.7
358.4	2.1
400.5	3.0
437.3	2.7
476.8	13.0
548.6	5.2
589.1	14.4
644.5	1.6
686.7	2.3
769.4	1.8
813.0	5.0
844.3	8.8
909.2	17.4
938.5	16.7
949.0	1.1
953.6	1.7
975.1	12.7
1013.2	15.3
1021.8	5.8
1052.3	1.7
1089.1	10.9
1105.5	23.0
1117.5	14.1
1160.3	27.6
1206.1	10.6
1218.2	42.8
1235.1	6.2
1239.2	14.1
1292.8	4.8
1311.8	0.8
1327.5	5.7
1335.8	7.8
1365.9	2.5
1399.8	16.5
1409.8	0.5
1413.6	6.6
1467.4	9.4
1486.1	1.2
1495.2	2.0
1498.9	15.0
1505.1	1.9
1509.5	2.8
1520.9	8.0
1524.6	6.9
3061.4	12.4
3079.4	21.0
3082.0	25.1
3088.0	11.7
3104.4	25.7
3138.3	12.2
3138.8	4.9
3145.5	28.6
3161.1	24.5
3171.7	12.4
3175.5	13.2
3178.9	16.3
3196.1	20.1
3827.7	26.6

Table S233: MP2 Frequencies and IR Intensities of cis-2-ethyl-2,3-epoxy-1-methylcyclopentan-1-ol (H-bonded) with the TZ basis set

Frequency	IR Intensity
93.6	0.1
100.6	2.8
170.1	0.6
199.0	0.4
225.6	1.6
270.4	0.3
296.1	1.6
309.6	0.9
354.8	2.0
394.5	7.5
430.2	27.2
444.5	36.4
477.0	43.3
550.9	6.8
594.7	10.4
648.3	3.4
682.4	3.6
770.3	2.1
812.0	2.2
838.6	8.5
914.9	10.8
931.8	13.3
950.4	1.7
959.3	7.1
972.7	19.2
1013.0	31.4
1024.8	2.1
1052.6	11.2
1090.3	4.7
1108.6	7.4
1122.9	9.8
1166.8	33.6
1179.7	6.0
1214.4	39.7
1237.9	7.2
1268.2	0.6
1296.4	9.6
1314.0	7.0
1331.9	1.7
1344.7	0.4
1368.8	4.8
1391.0	23.7
1413.4	6.3
1424.5	34.2
1471.8	8.1
1487.5	2.3
1493.5	2.8
1498.7	15.3
1502.1	0.1
1512.4	2.0
1521.1	6.4
1525.8	4.2
3074.8	8.3
3079.8	17.7
3082.3	20.8
3082.9	20.9
3109.7	16.6
3134.3	3.2
3138.8	17.2
3161.6	23.3
3167.5	14.3
3168.5	17.0
3175.0	20.9
3181.7	12.1
3195.9	19.3
3796.4	28.1

Table S234: MP2 Frequencies and IR Intensities of trans-2-ethyl-2,3-epoxy-1-methylcyclopentan-1-ol with the TZ basis set

Frequency	IR Intensity
48.9	0.0
123.3	1.8
175.3	1.4
217.8	0.9
228.8	3.8
263.7	9.9
268.4	20.6
280.2	56.7
304.9	4.1
371.4	7.7
391.7	3.8
427.6	1.6
471.8	14.0
542.1	5.7
589.6	2.6
642.7	2.7
695.4	0.3
775.3	2.2
812.4	4.5
852.4	6.2
887.8	2.2
939.3	25.7
943.9	4.0
958.7	23.7
986.9	2.7
1004.9	19.8
1029.1	8.9
1054.7	5.4
1089.7	15.8
1102.7	26.8
1121.1	3.1
1160.3	3.0
1206.1	7.9
1215.9	57.8
1235.6	1.8
1241.7	3.6
1289.3	4.5
1313.9	6.7
1333.7	5.4
1345.9	2.9
1361.8	1.1
1399.3	10.4
1411.8	1.2
1419.8	21.9
1468.8	4.9
1483.5	3.9
1492.0	4.9
1493.8	4.6
1505.5	4.9
1510.7	3.0
1514.1	6.6
1528.3	5.7
3063.1	14.8
3076.5	17.8
3080.5	29.4
3090.9	24.6
3103.6	24.9
3127.0	11.5
3146.2	9.6
3149.2	16.0
3159.0	29.6
3167.3	9.7
3173.8	17.0
3198.2	11.8
3199.4	14.0
3820.3	24.9

Table S235: MP2 Frequencies and IR Intensities of cis-2,3- thiirane-1,2-dimethylcyclopentan-1-ol (not H-bonded) with the TZ basis set

Frequency	IR Intensity
123.0	0.4
209.5	2.1
219.9	7.8
236.0	39.5
247.4	41.5
272.7	2.1
321.3	2.0
325.5	1.2
347.8	0.6
375.2	1.0
427.5	5.8
490.0	10.9
568.1	2.7
604.9	0.8
622.4	1.7
676.7	10.1
760.5	0.7
833.7	4.7
911.7	4.0
939.5	6.2
946.5	1.0
980.9	2.5
988.9	8.4
1015.9	7.4
1060.2	1.5
1074.2	17.2
1097.4	35.0
1138.8	16.0
1187.1	33.4
1203.8	13.2
1230.0	38.1
1237.5	5.7
1266.0	0.9
1322.1	10.4
1323.6	10.2
1372.3	0.3
1394.1	28.7
1401.7	2.9
1410.0	7.0
1483.6	4.6
1495.9	13.8
1497.1	7.0
1502.3	2.8
1509.6	5.0
1519.5	1.4
3062.5	11.5
3070.0	21.6
3072.1	27.2
3103.3	23.6
3140.3	14.6
3146.0	19.6
3155.1	10.8
3172.1	8.7
3175.6	7.4
3177.6	12.5
3196.4	7.2
3825.9	27.6

Table S236: MP2 Frequencies and IR Intensities of cis-2,3- thiirane-1,2-dimethylcyclopentan-1-ol (H-bonded) with the TZ basis set

Frequency	IR Intensity
119.8	3.0
211.4	0.9
229.2	0.1
233.4	0.2
264.9	0.6
314.1	0.6
319.3	0.6
342.1	1.4
371.4	2.4
419.6	21.0
435.4	62.0
497.7	20.8
568.9	5.0
599.6	0.1
623.9	4.2
674.4	7.9
754.6	1.1
830.6	2.3
912.8	0.2
944.8	2.2
953.8	3.6
979.4	14.4
991.0	4.0
1018.0	29.7
1058.6	7.6
1078.5	10.2
1102.0	5.5
1141.9	29.7
1169.1	9.4
1210.9	14.9
1232.1	41.4
1251.6	12.8
1269.8	0.7
1320.0	1.2
1336.6	6.8
1378.7	41.8
1392.1	15.5
1411.2	7.4
1414.8	23.5
1484.4	7.8
1491.0	4.5
1496.7	12.0
1501.6	5.4
1507.1	4.9
1521.5	0.5
3069.7	15.1
3072.9	18.7
3076.3	17.9
3110.2	13.1
3141.8	14.5
3154.9	8.5
3167.1	10.1
3168.1	16.6
3174.7	8.4
3181.5	11.9
3196.7	5.9
3775.5	19.0

Table S237: MP2 Frequencies and IR Intensities of trans-2,3- thiirane-1,2-dimethylcyclopentan-1-ol with the TZ basis set

Frequency	IR Intensity
121.3	1.1
213.0	1.0
221.3	1.9
239.0	4.1
252.4	0.3
262.6	79.3
289.4	9.5
324.1	2.3
333.6	2.8
385.6	5.2
407.9	2.8
458.5	2.1
578.2	6.3
610.1	0.3
627.1	3.1
679.5	21.3
774.0	6.3
828.6	2.5
901.6	7.2
931.8	7.5
943.8	19.6
978.5	5.1
995.1	0.7
1016.1	5.7
1062.3	19.0
1075.0	34.2
1092.4	8.1
1140.8	1.8
1180.9	31.1
1210.1	7.6
1227.7	0.9
1235.7	13.3
1259.4	11.2
1322.8	4.4
1340.7	4.5
1371.7	10.1
1397.2	7.9
1402.6	25.4
1408.8	3.5
1476.1	5.2
1491.4	6.3
1493.3	7.6
1502.1	3.6
1508.9	6.8
1511.1	3.1
3064.1	16.4
3076.0	17.5
3085.8	22.1
3101.7	23.6
3147.9	8.3
3149.7	17.4
3162.6	10.2
3166.1	10.5
3174.7	11.9
3178.1	6.7
3201.9	5.8
3820.7	26.5

Table S238: MP2 Frequencies and IR Intensities of cis-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) with the TZ basis set

Frequency	IR Intensity
73.6	0.2
123.5	0.1
176.4	0.3
201.6	79.7
221.6	1.6
228.7	4.2
271.3	14.1
285.1	2.6
323.3	1.3
341.9	2.3
345.0	0.4
366.6	0.8
423.6	7.2
514.8	6.8
567.0	2.6
613.7	2.4
641.3	0.3
677.1	12.0
741.0	1.2
794.6	1.6
834.6	4.4
911.7	3.4
937.4	4.0
959.4	6.6
989.3	9.5
1009.9	16.2
1019.4	4.7
1039.2	16.1
1068.4	6.6
1075.2	8.1
1107.0	12.9
1138.8	14.7
1183.0	11.2
1196.0	20.8
1224.3	37.0
1232.5	6.9
1267.9	1.1
1308.1	7.0
1319.5	9.5
1325.8	0.3
1355.7	5.8
1374.2	0.2
1396.5	21.7
1407.8	2.8
1419.0	8.4
1479.7	2.0
1486.1	13.9
1499.1	7.4
1505.0	3.0
1508.7	6.6
1516.1	4.7
1527.1	8.5
3069.3	7.0
3070.2	23.2
3073.5	17.9
3076.1	31.7
3116.1	18.5
3134.9	8.7
3139.8	11.7
3156.1	21.4
3157.7	7.0
3167.8	23.9
3174.7	8.3
3176.4	15.6
3195.5	7.5
3833.9	26.4

Table S239: MP2 Frequencies and IR Intensities of cis-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) with the TZ basis set

Frequency	IR Intensity
126.4	1.8
148.1	0.4
210.5	0.4
231.6	0.6
236.6	1.0
251.0	0.2
271.9	0.1
311.7	1.1
333.4	0.6
347.2	0.3
408.7	10.6
429.2	32.5
458.8	40.5
492.5	20.8
574.9	5.6
600.9	0.2
628.3	2.7
674.8	9.7
744.1	0.1
794.3	2.9
833.2	1.8
913.2	1.1
933.2	16.0
960.5	4.9
987.1	0.9
1004.7	10.9
1037.3	15.6
1059.5	27.1
1071.9	16.6
1080.8	7.4
1113.3	8.9
1139.5	13.4
1173.2	14.1
1191.7	21.6
1223.8	9.5
1242.8	2.8
1257.5	5.7
1312.8	1.6
1318.8	0.3
1325.8	1.0
1363.6	29.3
1392.6	13.6
1395.2	37.0
1411.4	5.1
1416.6	4.0
1483.4	4.5
1491.9	12.8
1497.4	9.4
1503.5	5.6
1511.2	1.9
1517.1	9.4
1527.8	3.6
3069.8	16.1
3074.6	11.7
3085.4	15.5
3089.5	29.1
3105.9	15.4
3132.9	4.0
3142.5	11.8
3154.3	14.9
3159.3	21.4
3162.4	20.8
3166.6	19.9
3173.3	6.6
3193.1	5.6
3764.0	19.4

Table S240: MP2 Frequencies and IR Intensities of trans-2,3-thiirane-1-ethyl-2-methylcyclopentan-1-ol with the TZ basis set

Frequency	IR Intensity
92.8	0.1
116.3	1.0
169.5	0.9
213.9	0.2
235.5	7.6
241.2	20.1
267.4	68.2
283.6	6.3
291.4	4.2
324.7	0.9
342.1	2.8
408.3	4.0
414.2	1.7
478.2	1.6
571.4	5.2
611.6	1.1
646.2	3.0
678.4	19.6
768.1	8.2
793.3	0.5
839.6	1.9
910.6	4.0
948.5	21.7
969.1	11.3
983.0	18.1
993.1	19.2
1016.4	5.9
1032.6	0.6
1067.2	6.8
1078.2	17.1
1104.6	2.9
1143.8	1.5
1181.1	28.0
1201.4	3.6
1225.3	1.8
1232.4	17.0
1255.7	7.9
1314.7	5.2
1316.8	3.0
1339.5	3.4
1346.1	5.2
1377.8	9.8
1398.7	17.5
1407.7	2.4
1418.8	3.5
1476.8	4.7
1486.3	6.4
1491.5	4.6
1494.9	4.4
1509.9	6.8
1516.3	6.9
1525.8	6.4
3069.8	16.6
3075.6	10.2
3078.8	23.1
3084.7	23.9
3101.6	20.8
3129.6	2.6
3146.5	9.1
3154.3	25.5
3162.6	11.6
3163.4	14.1
3165.9	21.4
3176.9	5.7
3201.0	6.2
3825.6	23.8

Table S241: MP2 Frequencies and IR Intensities of cis-2-ethyl-2,3-thiirane-1-methylcyclopentan-1-ol (not H-bonded) with the TZ basis set

Frequency	IR Intensity
83.9	0.2
109.0	0.5
185.5	1.0
205.9	0.6
228.8	5.3
245.8	78.0
275.3	5.1
290.2	2.6
329.9	1.8
346.8	1.1
360.5	1.4
379.8	1.0
439.0	4.5
497.0	9.9
563.5	2.4
614.3	2.7
630.1	0.7
710.2	10.0
748.4	1.2
802.3	4.1
835.9	7.9
909.6	9.5
943.8	2.0
948.1	0.8
966.0	6.8
994.4	5.2
1017.4	3.0
1025.6	5.1
1068.8	2.8
1085.9	11.7
1104.9	30.8
1139.0	17.3
1184.1	34.6
1203.0	13.6
1211.5	8.0
1228.9	26.8
1260.8	1.8
1314.7	2.9
1318.3	5.7
1322.2	13.4
1353.3	3.9
1376.4	0.5
1394.4	26.3
1399.9	0.8
1410.7	9.1
1483.2	4.9
1492.9	2.5
1497.9	14.0
1504.5	1.7
1509.4	5.6
1520.0	6.8
1523.4	5.6
3061.0	13.9
3069.8	26.4
3079.9	22.8
3087.1	11.0
3103.2	23.9
3139.0	14.5
3140.7	1.0
3144.9	28.2
3158.1	22.2
3172.9	8.4
3176.9	13.3
3185.4	16.2
3201.1	7.3
3824.1	26.8

Table S242: MP2 Frequencies and IR Intensities of cis-2-ethyl-2,3-thiiranene-1-methylcyclopentan-1-ol (H-bonded) with the TZ basis set

Frequency	IR Intensity
96.8	1.8
108.1	0.9
184.1	0.8
205.0	0.0
226.2	1.2
273.9	0.1
286.4	0.6
322.1	0.1
342.7	8.4
360.7	1.0
373.5	6.8
392.9	78.0
435.3	4.0
500.1	13.1
565.6	3.6
614.9	1.9
633.1	1.8
710.2	9.3
752.5	0.6
804.0	2.6
831.9	5.3
911.2	2.1
943.3	2.8
954.2	1.0
970.2	6.6
995.4	15.6
1020.9	18.9
1026.9	13.8
1069.3	9.4
1089.1	5.5
1101.5	9.0
1145.6	22.8
1164.5	8.0
1206.1	4.3
1224.3	24.7
1241.0	43.8
1250.7	1.1
1314.9	7.9
1317.5	4.2
1338.7	2.4
1352.5	1.3
1373.0	48.6
1391.5	5.5
1410.0	18.5
1412.3	8.5
1484.1	6.1
1490.5	1.8
1496.7	17.0
1501.2	0.0
1512.5	4.4
1520.5	5.7
1525.5	2.8
3069.8	10.3
3071.1	19.7
3074.5	24.4
3082.4	11.9
3110.1	13.1
3137.8	2.4
3142.9	16.2
3153.3	21.7
3164.0	15.6
3166.3	15.0
3172.2	17.5
3180.4	12.2
3203.5	6.3
3809.1	20.7

Table S243: MP2 Frequencies and IR Intensities of trans-2-ethyl-2,3-thiirane-1-methylcyclopentan-1-ol with the TZ basis set

Frequency	IR Intensity
53.1	0.1
115.3	0.9
185.7	0.8
215.0	0.1
225.8	2.4
254.9	0.4
266.5	0.5
278.1	73.8
296.7	14.5
326.4	1.6
363.0	5.4
401.5	6.2
404.8	1.9
473.0	3.9
572.2	5.9
615.9	0.9
630.6	1.6
709.2	17.1
764.4	3.4
806.5	16.5
832.0	0.7
898.2	11.6
936.1	2.3
949.9	19.6
969.2	1.7
994.8	10.1
1014.3	1.6
1034.1	4.0
1069.2	0.4
1092.5	35.2
1098.3	12.8
1141.2	1.8
1179.3	26.6
1207.2	6.4
1210.9	1.4
1231.2	11.9
1253.9	9.9
1316.0	10.0
1319.7	4.2
1339.2	2.8
1352.6	1.0
1380.1	3.9
1395.8	1.0
1403.1	19.0
1407.8	18.7
1475.5	4.7
1487.9	5.8
1491.3	5.3
1502.5	4.0
1507.5	2.5
1509.7	7.6
1526.8	4.2
3063.2	16.3
3078.4	27.6
3081.1	17.1
3083.1	22.1
3102.0	23.1
3132.0	8.4
3146.6	10.5
3148.6	16.0
3154.5	29.7
3166.6	9.8
3176.3	12.8
3201.7	4.7
3206.4	6.7
3814.2	24.9

Table S244: MP2 Frequencies and IR Intensities of cis-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol (not H-bonded) with the TZ basis set

Frequency	IR Intensity
114.4	3.1
153.0	88.9
203.7	1.7
225.5	1.2
235.7	2.2
278.4	1.3
301.5	0.7
317.6	1.4
346.1	0.0
372.3	0.8
421.9	2.3
472.2	8.5
556.2	1.4
587.7	0.2
600.6	0.9
653.2	0.7
719.1	1.3
754.8	1.7
831.5	3.8
887.7	8.3
916.9	11.1
941.7	8.2
955.9	0.4
974.5	0.1
989.1	7.9
1011.9	7.6
1056.6	5.1
1081.6	23.3
1098.5	21.8
1135.8	22.1
1168.8	29.7
1199.7	9.8
1225.3	36.4
1233.6	10.3
1258.7	2.9
1314.4	24.8
1321.2	2.8
1359.9	2.7
1387.2	23.0
1397.1	7.7
1406.9	4.8
1490.2	2.8
1497.6	4.4
1501.1	11.5
1507.2	10.8
1510.6	1.3
1521.7	1.4
2441.4	73.2
3055.3	13.6
3057.0	31.0
3070.6	33.1
3088.0	13.0
3132.9	17.0
3136.0	14.1
3140.9	20.9
3147.7	24.4
3160.8	11.6
3168.7	12.2
3207.1	5.3
3856.5	26.4

Table S245: MP2 Frequencies and IR Intensities of cis-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol (H-bonded) with a TZ basis set

Frequency	IR Intensity
118.9	2.9
202.3	1.7
224.8	0.0
233.6	0.2
263.3	6.3
300.8	0.8
311.6	8.2
318.0	61.0
344.0	7.6
372.6	3.3
421.5	2.1
470.4	11.1
558.6	1.8
586.8	0.2
601.7	5.2
647.1	1.2
717.0	1.4
749.4	1.1
827.5	0.4
879.2	8.3
921.9	1.4
946.5	2.7
960.4	3.7
974.9	0.5
989.5	8.6
1010.8	45.3
1054.9	3.4
1086.9	8.1
1094.4	8.0
1136.0	32.4
1163.3	6.2
1204.4	6.8
1229.6	56.4
1240.5	14.9
1255.3	2.2
1317.7	3.1
1329.3	8.3
1370.2	47.0
1377.8	9.1
1407.7	10.2
1408.9	17.7
1489.7	5.7
1491.6	2.7
1501.5	12.4
1506.5	10.8
1508.3	1.2
1523.6	0.9
2453.5	62.6
3057.3	24.5
3070.3	9.6
3074.0	31.3
3085.0	10.7
3137.0	19.1
3137.7	11.8
3152.9	19.0
3159.9	11.4
3163.0	17.1
3174.7	12.4
3205.9	4.8
3820.0	17.1

Table S246: MP2 Frequencies and IR Intensities of trans-2,3-phosphirane-1,2-dimethylcyclopentan-1-ol with the TZ basis set

Frequency	IR Intensity
117.4	7.8
139.5	88.2
208.1	1.6
213.3	0.2
238.3	1.0
259.6	0.3
288.5	1.8
312.0	0.8
320.0	2.7
379.6	4.3
403.4	2.3
445.1	2.3
557.7	1.8
603.1	4.2
604.9	0.5
652.4	9.6
722.1	1.4
772.0	2.7
818.3	7.5
885.8	7.9
905.5	6.3
944.1	0.6
952.4	24.6
976.0	11.4
989.0	2.0
1014.1	4.6
1060.1	3.6
1073.4	56.9
1093.4	0.5
1136.7	1.9
1167.7	28.9
1205.3	4.8
1219.9	0.8
1234.7	13.4
1252.5	23.3
1314.0	4.4
1335.0	2.3
1358.3	10.0
1385.6	9.7
1402.2	20.1
1406.1	7.6
1482.6	4.8
1494.1	7.0
1498.2	4.1
1502.1	3.6
1508.4	2.6
1514.1	8.4
2446.0	67.0
3055.7	18.3
3064.0	25.7
3083.4	16.5
3086.1	26.4
3136.9	10.3
3141.0	25.2
3147.9	13.9
3148.7	18.2
3160.7	8.1
3165.9	13.9
3211.1	4.4
3855.5	25.5

Table S247: MP2 Frequencies and IR Intensities of cis-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) with the TZ basis set

Frequency	IR Intensity
78.6	1.4
108.5	91.4
125.0	5.1
170.5	0.4
222.1	1.5
227.2	0.3
266.8	3.5
282.1	2.7
306.2	0.9
331.7	2.4
340.4	0.8
361.0	0.3
419.7	2.5
497.3	6.0
554.4	1.6
584.6	0.5
630.5	1.1
659.1	0.8
718.9	1.7
733.5	0.6
796.3	1.3
830.1	4.3
889.1	7.9
918.7	12.3
940.3	5.4
960.5	4.7
982.6	4.9
1006.6	18.7
1017.6	2.6
1044.0	19.6
1063.4	5.6
1084.4	7.1
1107.2	11.6
1135.2	20.4
1168.4	14.7
1189.6	9.0
1220.4	41.9
1228.9	3.9
1262.6	2.9
1298.6	21.5
1310.7	4.1
1326.0	0.2
1350.8	8.2
1364.8	0.9
1389.6	19.4
1406.3	5.1
1416.3	3.5
1480.5	2.8
1493.8	10.4
1504.3	7.0
1507.6	2.1
1513.2	8.2
1516.9	5.1
1527.9	9.0
2442.3	74.5
3057.1	25.5
3066.4	10.7
3068.0	25.9
3072.1	33.0
3094.4	9.9
3129.2	8.6
3133.9	16.0
3138.8	13.3
3149.0	15.5
3154.2	29.2
3160.7	15.0
3163.1	25.6
3206.3	5.7
3863.6	25.3

Table S248: MP2 Frequencies and IR Intensities of cis-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) with the TZ basis set

Frequency	IR Intensity
121.6	1.7
145.6	0.2
217.4	0.2
221.1	1.0
229.8	0.2
248.5	0.5
285.4	0.1
307.2	7.0
311.9	57.6
326.8	16.3
345.7	1.3
409.4	4.1
436.8	7.0
465.0	5.5
564.2	1.4
590.8	0.4
597.2	3.7
653.8	1.3
715.4	1.4
736.2	2.1
795.7	2.1
828.3	0.6
878.4	8.8
923.2	4.9
934.9	8.9
960.4	3.0
978.4	10.6
1005.0	8.1
1035.0	20.9
1058.9	10.2
1075.6	31.9
1083.5	9.4
1105.3	9.2
1136.9	18.6
1166.2	9.7
1189.3	16.7
1216.8	17.1
1233.9	6.1
1247.2	5.4
1306.8	2.1
1315.3	0.8
1319.7	3.0
1359.3	41.6
1380.4	17.9
1382.9	11.5
1407.0	9.8
1416.5	3.8
1486.7	3.1
1495.3	12.2
1500.6	9.3
1505.5	5.5
1515.7	5.6
1517.2	8.0
1530.7	3.1
2453.7	61.2
3057.6	24.7
3064.8	13.1
3082.9	16.0
3086.1	13.5
3091.5	32.1
3127.9	1.7
3137.1	17.1
3137.2	11.1
3148.2	19.2
3150.3	40.7
3158.2	16.0
3159.2	13.9
3202.9	4.2
3816.9	16.7

Table S249: MP2 Frequencies and IR Intensities of trans-2,3-phosphirane-1-ethyl-2-methylcyclopentan-1-ol with the TZ basis set

Frequency	IR Intensity
91.9	3.7
114.6	17.9
134.3	80.5
170.0	3.2
211.5	0.2
227.4	0.5
254.0	2.6
282.6	2.3
291.1	1.2
312.4	0.4
333.8	3.7
401.3	2.2
409.4	1.9
458.4	1.3
551.7	2.3
597.4	3.7
635.0	0.8
649.9	8.4
722.3	1.6
766.8	3.4
793.2	1.9
831.6	6.4
883.7	6.7
922.3	6.7
948.8	6.3
975.0	11.1
978.0	11.6
989.9	46.9
1014.4	3.0
1032.4	1.9
1063.6	2.4
1085.8	21.7
1102.5	1.2
1138.9	1.4
1168.4	25.0
1197.0	2.6
1219.0	1.6
1231.9	19.1
1247.4	15.3
1302.7	8.2
1314.8	2.2
1334.7	2.6
1341.2	5.4
1365.4	5.3
1392.1	15.5
1404.7	6.9
1415.5	3.1
1483.3	3.7
1486.3	5.5
1495.8	4.2
1498.1	4.1
1513.5	8.5
1517.1	6.6
1527.1	5.7
2445.4	68.4
3061.0	18.3
3064.1	22.4
3074.2	19.3
3080.8	12.8
3084.9	28.2
3122.3	2.0
3136.3	16.1
3145.9	32.2
3147.3	15.1
3148.8	16.9
3156.6	22.6
3159.9	9.2
3210.4	4.7
3861.2	23.0

Table S250: MP2 Frequencies and IR Intensities of cis-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol (not H-bonded) with the TZ basis set

Frequency	IR Intensity
88.8	1.2
111.9	0.5
157.7	87.0
193.5	3.0
204.6	0.7
222.6	1.9
280.0	2.3
286.1	1.1
307.5	0.4
347.4	0.3
355.7	2.8
374.0	0.3
438.0	1.4
481.0	7.0
552.8	1.7
590.4	0.4
615.8	0.7
687.0	1.0
718.2	1.1
746.0	3.9
796.1	2.7
832.9	4.7
896.0	12.1
913.3	17.0
946.8	0.8
958.6	0.4
963.0	3.6
992.8	1.0
1011.2	8.7
1022.4	1.3
1067.4	2.3
1084.2	15.1
1102.3	24.8
1135.3	25.3
1166.3	27.9
1199.3	1.8
1202.6	23.0
1229.4	28.6
1252.5	5.0
1309.5	17.0
1313.6	5.0
1318.3	7.7
1350.4	2.7
1363.6	6.3
1381.5	18.4
1398.3	9.7
1409.7	7.3
1488.7	2.0
1493.7	4.8
1502.2	11.3
1507.3	5.2
1511.4	3.5
1518.6	6.8
1522.7	4.2
2439.2	72.5
3055.3	16.4
3068.8	32.7
3071.7	24.9
3081.5	14.1
3088.6	13.1
3129.5	4.1
3132.5	17.6
3139.6	29.4
3147.9	23.1
3150.1	25.4
3169.2	12.2
3173.7	18.7
3212.0	5.0
3856.6	25.7

Table S251: MP2 Frequencies and IR Intensities of cis-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol (H-bonded) with TZ basis

Frequency	IR Intensity
95.2	1.1
113.1	1.2
192.4	1.0
203.1	0.3
219.2	0.7
273.7	3.3
284.4	0.7
304.2	2.4
323.5	49.5
345.5	29.3
352.6	0.3
375.2	3.1
436.1	1.8
478.5	9.3
556.1	2.0
590.5	0.7
616.2	4.6
681.3	1.5
715.5	1.4
743.1	1.8
795.6	3.0
828.7	0.4
887.6	10.9
919.7	3.8
950.5	0.4
957.9	0.8
968.5	4.7
992.6	4.7
1009.0	40.5
1023.5	6.9
1066.0	3.3
1088.6	2.3
1097.7	13.5
1139.8	25.2
1161.8	7.6
1199.3	1.4
1217.9	30.4
1231.0	43.6
1243.7	5.6
1311.2	2.5
1316.2	14.0
1332.9	1.0
1351.4	3.2
1370.0	30.9
1373.5	22.3
1408.0	23.4
1410.0	7.6
1488.3	2.9
1491.8	5.1
1498.2	13.0
1506.3	3.7
1513.3	4.5
1517.6	5.1
1524.4	2.8
2454.3	61.5
3070.5	10.3
3072.3	15.3
3073.0	38.3
3079.1	13.9
3086.9	10.0
3127.8	5.3
3136.5	19.9
3151.0	23.2
3152.8	19.3
3164.0	24.1
3172.7	14.1
3177.1	12.3
3209.7	4.6
3818.0	17.4

Table S252: MP2 Frequencies and IR Intensities of trans-2-ethyl-2,3-phosphirane-1-methylcyclopentan-1-ol with the TZ basis set

Frequency	IR Intensity
78.2	0.3
105.6	1.9
160.8	85.6
198.5	5.1
209.9	1.0
214.2	1.1
258.4	0.3
280.4	0.4
287.9	2.6
305.6	0.2
353.6	4.3
391.1	2.5
407.2	2.9
466.1	4.0
554.1	1.9
603.8	3.1
612.7	0.4
684.0	7.3
720.7	2.3
753.1	1.9
808.0	12.9
817.5	4.6
895.5	9.0
900.7	9.7
948.5	3.6
961.4	15.6
963.5	4.2
997.3	6.8
1009.1	4.3
1030.1	1.9
1066.4	1.2
1084.5	36.0
1099.9	11.9
1135.9	2.9
1164.2	23.2
1200.1	4.6
1203.0	3.0
1230.5	10.0
1247.2	27.7
1309.7	5.6
1316.5	8.5
1333.5	1.6
1352.0	1.6
1361.8	6.3
1380.4	9.1
1403.7	4.9
1405.9	26.6
1481.3	5.4
1485.8	4.4
1497.5	4.4
1501.8	4.9
1506.3	1.7
1510.0	7.9
1525.6	3.0
2447.2	65.0
3055.2	18.4
3070.4	31.2
3079.7	19.6
3082.1	29.1
3084.0	13.6
3125.8	10.1
3137.2	9.5
3140.3	24.8
3147.4	29.5
3147.6	21.8
3167.7	13.2
3188.0	7.5
3215.3	4.0
3851.0	23.6

Table S253: MP2 Frequencies and IR Intensities of cis-2,3-aziridine-1,2-dimethylcyclopentan-1-ol (not H-bonded) with the TZ basis set

Frequency	IR Intensity
80.7	93.4
133.5	7.9
214.2	3.3
217.8	0.1
241.2	0.8
277.6	0.5
320.7	0.6
360.1	1.6
374.6	0.9
417.9	4.9
466.5	8.9
512.8	15.7
580.2	3.9
648.9	1.5
662.4	2.7
805.7	1.7
844.1	1.3
861.2	29.6
926.1	6.8
942.9	12.2
950.9	12.4
969.9	8.5
1000.5	19.1
1013.7	14.1
1042.4	16.0
1085.9	31.3
1091.5	1.1
1120.6	38.9
1146.8	21.5
1159.6	13.1
1206.8	17.9
1236.9	26.3
1239.5	10.0
1290.3	15.2
1311.5	12.3
1331.7	1.4
1346.6	7.4
1397.8	22.8
1407.3	3.2
1412.3	6.4
1466.5	5.2
1484.3	4.8
1497.9	9.4
1500.1	8.2
1504.6	0.9
1513.2	6.3
1525.8	1.6
3056.2	13.7
3061.4	21.9
3080.2	29.6
3099.4	29.7
3135.3	18.6
3140.7	23.3
3148.1	13.9
3152.0	14.8
3164.6	15.1
3171.5	11.1
3200.1	16.4
3544.8	1.8
3859.2	25.8

Table S254: MP2 Frequencies and IR Intensities of cis-2,3-aziridine-1,2-dimethylcyclopentan-1-ol (H-bonded) with the TZ basis set

Frequency	IR Intensity
106.1	2.7
217.9	0.4
226.2	0.3
230.6	1.0
274.3	0.9
313.1	1.2
348.0	7.2
368.2	2.4
417.3	17.2
428.7	55.4
466.7	26.0
517.4	15.3
588.8	3.7
653.7	7.8
658.7	1.6
804.7	0.1
836.0	0.7
867.5	19.0
926.8	12.5
940.5	12.6
958.8	9.6
975.4	2.6
1001.1	30.4
1019.1	29.2
1041.4	20.6
1089.2	7.1
1103.4	10.4
1128.9	15.9
1129.9	13.8
1177.3	3.4
1196.3	17.6
1223.3	69.1
1250.0	1.3
1301.2	9.4
1331.9	2.6
1344.8	0.9
1351.4	5.0
1387.7	34.1
1410.7	10.0
1422.2	33.4
1471.1	4.2
1486.3	7.9
1495.2	4.1
1499.2	9.6
1504.9	1.8
1512.5	5.8
1526.8	1.4
3058.8	20.7
3066.5	11.8
3080.4	30.5
3106.6	18.1
3134.8	19.0
3144.5	12.6
3151.8	13.3
3158.9	16.8
3164.5	16.4
3169.2	16.6
3200.1	16.5
3541.6	2.1
3814.0	26.7

Table S255: MP2 Frequencies and IR Intensities of trans-2,3-aziridine-1,2-dimethylcyclopentan-1-ol with the TZ basis set

Frequency	IR Intensity
120.2	4.5
160.4	95.0
215.2	1.7
227.9	3.9
245.1	0.8
268.7	0.8
284.9	2.5
346.3	0.2
377.5	5.5
422.2	0.9
460.6	16.9
492.2	1.2
594.8	4.2
642.6	0.1
675.1	0.4
807.7	3.0
843.0	4.1
861.9	17.8
920.4	7.4
941.5	26.0
955.6	6.9
964.2	23.6
1003.3	20.7
1017.4	24.2
1038.7	18.4
1087.0	27.6
1093.6	5.4
1124.6	4.7
1135.1	6.4
1164.5	5.9
1208.4	6.1
1232.7	74.7
1240.4	4.3
1290.2	13.2
1313.5	6.0
1342.3	1.2
1350.6	2.5
1397.5	12.4
1405.9	11.1
1415.1	11.2
1470.0	3.6
1478.6	5.6
1494.5	7.6
1496.3	4.9
1504.4	3.0
1513.8	3.8
1522.4	4.2
3054.6	19.2
3059.0	26.0
3088.8	29.7
3099.1	29.8
3136.7	22.9
3140.1	15.2
3143.2	11.9
3162.3	3.4
3166.6	22.9
3170.2	7.2
3204.5	15.8
3541.6	2.0
3861.9	26.6

Table S256: MP2 Frequencies and IR Intensities of cis-2,3-aziridine-1-ethyl-2-methylcyclopentan-1-ol (not H-bonded) with the TZ basis set

Frequency	IR Intensity
−160.6	111.6
85.9	0.7
130.9	0.3
182.8	0.4
216.7	1.1
226.3	1.0
269.3	3.0
290.9	0.7
324.2	0.5
355.4	0.5
380.8	1.6
420.9	8.0
471.1	3.7
526.7	14.5
581.8	2.5
643.9	2.2
687.9	2.1
788.6	1.2
797.4	2.1
846.2	0.9
861.0	29.4
927.4	12.5
949.1	1.9
967.2	39.2
975.0	16.5
1008.7	15.5
1021.3	2.3
1042.6	17.7
1050.2	25.0
1093.0	2.8
1100.2	7.1
1119.0	36.6
1145.1	14.4
1157.2	4.2
1191.0	7.8
1229.0	28.1
1249.6	11.1
1273.1	22.9
1302.0	0.3
1321.6	2.8
1336.1	0.9
1349.4	6.0
1363.4	7.7
1398.6	9.0
1410.7	5.4
1416.1	4.8
1467.2	5.3
1482.5	3.2
1485.7	10.9
1500.2	6.8
1504.3	2.4
1518.7	5.6
1520.7	6.3
1527.1	6.3
3061.4	17.0
3066.0	12.6
3068.8	28.1
3080.6	32.5
3111.0	23.4
3123.6	8.5
3135.7	17.9
3147.0	14.1
3152.5	26.6
3155.2	2.7
3158.7	37.1
3172.7	13.7
3199.8	16.9
3545.6	1.7
3870.0	27.1

Table S257: MP2 Frequencies and IR Intensities of cis-2,3-aziridine-1-ethyl-2-methylcyclopentan-1-ol (H-bonded) with the TZ basis set

Frequency	IR Intensity
78.7	1.5
123.7	1.1
180.7	1.0
220.9	0.6
230.2	0.1
243.4	1.6
284.4	2.5
316.6	1.4
348.2	3.8
377.8	5.6
417.7	71.4
422.4	10.0
469.1	11.1
529.5	16.4
590.1	2.5
647.9	7.7
686.0	1.4
791.6	0.4
799.9	0.4
838.4	1.2
867.1	17.0
927.6	17.3
948.7	5.4
969.4	57.8
986.2	1.9
1014.8	13.9
1031.1	9.9
1040.9	15.0
1050.0	17.4
1095.9	6.6
1103.2	11.3
1128.0	5.4
1130.5	19.7
1168.5	7.6
1189.6	6.3
1214.0	59.6
1247.7	1.4
1291.2	5.3
1320.5	1.9
1332.5	6.2
1338.7	1.8
1352.1	3.3
1362.3	18.9
1410.3	7.2
1412.1	18.3
1416.8	21.2
1471.1	4.6
1483.2	7.3
1487.1	6.8
1500.0	5.7
1503.5	2.2
1518.0	7.8
1520.5	6.3
1524.6	5.5
3058.7	16.8
3062.4	21.9
3076.3	25.0
3079.8	30.6
3115.0	13.8
3119.1	11.7
3135.3	19.8
3144.0	14.0
3153.3	8.6
3157.5	38.8
3171.7	4.6
3175.8	23.3
3199.7	16.9
3541.7	2.0
3815.6	29.0

Table S258: MP2 Frequencies and IR Intensities of trans-2,3-aziridine-1-ethyl-2-methylcyclopentan-1-ol with the TZ basis set

Frequency	IR Intensity
99.6	1.4
122.3	23.2
145.4	79.8
172.6	3.9
215.9	0.5
246.2	1.7
256.2	1.4
276.7	5.2
294.8	1.5
357.3	0.5
400.5	1.4
428.2	3.1
473.1	14.2
497.9	2.5
581.3	3.2
662.9	0.6
683.3	0.3
791.6	3.7
819.8	1.8
839.3	5.1
863.7	17.7
928.1	13.9
961.0	0.7
964.5	37.3
986.5	23.4
995.9	44.8
1017.7	16.5
1037.5	0.5
1042.3	8.7
1092.3	1.5
1103.3	8.2
1123.5	5.5
1133.8	6.6
1167.6	4.2
1201.5	4.9
1223.6	63.6
1242.0	5.7
1274.0	22.1
1310.7	6.5
1322.9	0.5
1337.8	0.8
1350.3	2.2
1360.7	3.6
1404.6	15.6
1409.5	1.8
1421.7	8.1
1471.4	2.6
1479.1	4.6
1489.0	7.3
1495.7	2.9
1497.7	3.8
1517.6	6.0
1521.1	6.2
1525.5	5.2
3059.1	23.2
3059.8	17.7
3071.0	23.2
3088.0	32.2
3097.5	26.5
3121.3	1.5
3137.4	22.3
3141.7	10.6
3143.8	26.3
3156.6	25.3
3160.7	18.3
3169.6	6.2
3204.0	16.5
3541.5	1.9
3868.2	23.5

Table S259: MP2 Frequencies and IR Intensities of cis-2-ethyl-2,3-aziridine-1-methylcyclopentan-1-ol (not H-bonded) with the TZ basis set

Frequency	IR Intensity
79.6	64.3
94.2	20.8
118.5	13.1
190.8	2.3
213.4	0.6
233.6	0.8
278.9	2.3
301.9	0.6
336.7	0.6
361.9	1.3
405.6	4.1
435.5	3.1
470.0	12.2
536.3	5.5
587.8	8.0
640.2	1.5
670.3	4.1
768.9	2.5
811.0	3.8
856.4	4.6
873.7	25.5
931.7	40.3
939.0	3.4
961.7	7.1
978.6	2.4
1002.9	3.0
1013.9	13.6
1018.1	11.7
1068.9	12.9
1090.2	16.6
1105.1	8.4
1113.4	6.4
1139.5	67.3
1156.1	6.3
1207.1	17.1
1234.8	23.5
1236.9	12.1
1259.9	8.1
1307.3	9.8
1321.3	4.8
1328.6	3.7
1344.5	8.7
1363.4	2.8
1399.3	19.5
1410.5	3.1
1416.3	9.5
1459.5	3.6
1483.2	3.9
1492.4	4.5
1499.4	11.7
1505.5	1.0
1510.5	4.2
1520.1	7.8
1524.6	4.3
3054.2	13.5
3068.4	19.4
3071.6	24.9
3079.2	29.6
3099.4	29.5
3114.0	7.8
3134.6	18.8
3138.8	32.3
3151.6	26.3
3160.8	15.6
3170.8	16.6
3172.2	11.1
3200.0	16.0
3546.4	1.7
3858.6	25.6

Table S260: MP2 Frequencies and IR Intensities of cis-2-ethyl-2,3-aziridine-1-methylcyclopentan-1-ol (H-bonded) with the TZ basis set

Frequency	IR Intensity
96.0	1.8
105.0	0.5
173.2	0.6
212.5	0.5
232.6	1.2
275.2	0.3
296.4	2.5
332.1	1.2
356.5	2.9
399.0	6.5
435.1	5.4
439.9	52.7
472.2	44.5
538.4	5.9
595.5	5.4
644.9	7.1
668.8	4.8
772.0	2.6
811.9	1.1
851.4	2.4
881.9	14.0
928.2	36.0
940.4	4.0
966.4	13.6
980.7	3.3
1007.1	3.3
1014.6	24.5
1024.3	27.2
1068.8	16.5
1096.5	5.7
1104.6	15.4
1118.4	1.6
1133.9	15.2
1172.8	7.0
1195.3	18.5
1223.1	71.5
1246.3	1.0
1273.0	0.2
1311.7	11.7
1328.4	5.9
1341.4	1.4
1356.0	9.4
1365.6	3.7
1393.1	25.3
1414.2	7.4
1422.5	38.6
1465.2	2.9
1485.6	4.5
1490.5	4.6
1497.4	12.5
1503.2	1.1
1512.9	3.2
1520.6	5.3
1526.5	2.7
3060.7	21.5
3065.9	10.4
3072.8	24.6
3079.2	30.3
3107.1	11.4
3107.9	17.3
3134.2	20.3
3152.4	25.2
3160.3	17.5
3163.0	14.8
3166.8	23.2
3175.9	12.1
3197.0	16.2
3544.1	2.1
3810.3	27.6

Table S261: MP2 Frequencies and IR Intensities of trans-2-ethyl-2,3-aziridine-1-methylcyclopentan-1-ol with the TZ basis set

Frequency	IR Intensity
58.8	0.2
121.2	2.8
171.3	34.8
193.8	61.3
228.3	0.8
229.8	3.8
268.6	0.1
278.7	0.5
302.9	0.9
371.8	3.8
393.4	3.9
430.5	0.5
462.6	16.4
531.2	2.9
590.4	4.2
635.8	0.8
681.7	1.0
773.2	2.8
812.5	4.0
858.3	3.8
876.3	16.8
922.1	19.9
935.7	32.5
959.9	20.0
985.4	0.6
1001.5	3.9
1017.4	27.1
1024.9	9.1
1074.9	10.3
1086.4	28.9
1105.2	8.8
1122.1	2.6
1131.2	0.3
1163.3	7.8
1205.2	6.2
1231.0	80.4
1238.0	1.7
1263.7	3.1
1308.4	13.1
1321.8	8.0
1342.2	3.1
1348.8	2.1
1362.6	3.1
1397.0	14.4
1411.8	8.0
1420.6	11.2
1462.4	2.0
1478.6	5.1
1485.0	5.0
1495.7	4.4
1504.9	2.9
1509.0	4.7
1513.0	4.7
1528.4	4.0
3053.8	23.3
3055.5	23.3
3071.6	29.6
3087.5	29.5
3099.1	26.3
3102.0	24.2
3139.6	17.3
3142.3	13.9
3148.9	32.3
3163.9	4.3
3168.3	22.1
3194.9	5.7
3199.7	15.6
3545.7	2.0
3856.4	25.0

VITA

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Chemistry instructor and laboratory manager with 8+ years of experience in chemical investigation, instruction and training of laboratory techniques, laboratory safety protocol and compliance. Specializing in computation/theoretical chemistry with expert knowledge of various computer software for data analysis and report writing as well as laboratory safety operation and compliance. Possess a Bachelor of Arts in Biology and Psychology with a minor in Chemistry and Master of Arts in Higher Education Administration with a strong desire for education and establishing service projects that benefit neighboring communities, schools and student activities.

Education:

The University of Mississippi – *University, MS*

2011 Master of Arts in Higher Education Administration

2009 Bachelor of Arts in Biology and Psychology

Work Experience:

The University of Mississippi – Department of Chemistry & Biochemistry – *University, Mississippi*

Instructor/Laboratory Manager: August 1, 2011 – present

- Established and carried out efficient means of ordering all chemicals, gas cylinders,

cryogens, instrumentation and all other office and chemical supplies for the Department of Chemistry & Biochemistry

- Coordinated with research and instructional principal investigators for proper funding assignment of grants for all purchases
- Ensured all purchases are received in good condition and ready to be used in the chemistry laboratory setting
- Served as Chair of the Chemical Hygiene Committee for the Department of Chemistry, providing annual safety inspections
- Coordinated repairs with Facilities Management for all electrical, water, air, HVAC, door locks, alarms and networking components within the Department of Chemistry & Biochemistry
- Planned and organized weekly laboratory experiments for general and organic undergraduate laboratories
- Lectured and trained graduate teaching assistants on chemicals, reactions, and safety methods within the laboratory
- Supervised 50+ Teaching Assistants within the active laboratory and assisted students with operational research methods
- Ensured purity of chemicals used in the laboratory and coordinated safe disposal of hazardous chemicals and waste
- Calibrated and synchronized necessary equipment for chemical investigation including gas chromatographs, nuclear magnetic spectrometers, photo-spectrometers, pH meters and the computers and software that control instrumentation
- Assisted in the development of new experiments by utilizing standards, methods, and procedures learning in the classroom

- Represented the Department of Chemistry at all Visit Days, Job Fairs and community events to share program and curriculum information with prospective students, parents and the surrounding community.

The University of Mississippi – Department of Chemistry & Biochemistry – *University, Mississippi*

Graduate Researcher: August 1, 2015 – July 31, 2019

- Investigated electronic structure, energetics, and various intrinsic properties of chemical molecules using Linux-based software on the University of Mississippis supercomputer
- Drafted reports and published scientific research articles on chemical structures of interest, particular hydrogen bonding and non-covalent interactions
- Demonstrated understanding of chemical research via official reports and presentation in academic and convention settings
- Maintained hardware and software on computer cluster funded by federal research grants

The University of Mississippi – Office of Enrollment Services and Dean of Students – *University, Mississippi*

Graduate Assistant: August 1, 2009 – May 31, 2011

- Created new service programs for student rehabilitation with the surrounding community by establishing new community service projects and joint ventures for students on academic or disciplinary probation as well as students seeking completion of community service hours.
- Planned and coordinated visits for prospective students and families, including information sessions and tours of the university

- Prepared literature by analyzing current student and visiting student surveys based on their experience at the university
- Maintained prospective student contact information database in order to efficiently reach out to prospective students based on their academic and student organization interests
- Attended and added student perspective to meetings involving student organization and student satisfaction with academic programs

Knowledge, Skills and Abilities:

- Moderate experience in use and maintenance of scientific equipment including: gas chromatograph mass spectrometers, nuclear magnetic resonance spectrometers, matrix-assisted laser desorption ionization mass spectrometers, infrared and near-infrared spectrometers and photo-spectrometers
- Preparation of chemical standards to be used by researchers and undergraduate students
- Supervision of chemical investigators including graduate and undergraduate researchers
- Safety and chemical hygiene inspection and upkeep of chemical laboratories
- Purchasing and inventory control of chemicals, cryogens, gas cylinders and other laboratory equipment including large purchase orders with chemical companies including Fisher, VWR, Sigma-Aldrich and various others
- Data management, analysis and report creation for various projects and presentations requiring compilation, extraction and interpretation of scientific data
- Academic and career advising of undergraduate students by planning future coursework and career aspiration preparation

- Team player and coordinator of research for purchase orders and grant preparation
- Community service and joint venture liaison for academic programs involving prospective students, undergraduate and graduate students and Boy Scouts seeking to earn the Chemistry Merit Badge
- Proficient in Microsoft Suite (Excel, Word, Powerpoint)
- Proficient on Mac, Windows and Linux operating systems

Published Work:

Smith, B.E.; Carr, J.M.; Tschumper, G.S. *Cis/Trans* Energetics in Epoxide, Thiirane, Aziridine and Phosphirane Containing Cyclopentanols: Effects of Intramolecular OH$\cdots$O, S, N and P Contacts. *Molecules* 2019, *24*, 2523.

Honors and Activities:

- Alpha Lambda Delta Honors Society
- Phi Kappa Phi Outstanding Scholarship Honor Society
- Affiliate of the American Chemical Society
- Member of Pi Kappa Alpha Fraternity
- Member of First Presbyterian Church of Tupelo, MS
- Recipient of the Thomas "Sparky" Reardon Excellence in Student Services Award
- Nominated for 2018 Academic Advisor of the Year - University of Mississippi