

Supplementary Material

Qualitative and Quantitative Measurements of Hydrogen Bond-Mediated Scalar Couplings in Acyclic 1,3-Diols

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1. Pulse sequence for measuring small coupling constants.

All of the experiments using the selective spin echo pulse sequence shown in Figure 1 of the paper were performed on a Bruker Avance 300 MHz spectrometer equipped with a 5 mm broadband observe z -gradient probe. The temperature was maintained at 21.0 (± 0.1) °C for all selective spin-echo measurements. The samples were made by dissolving 0.5 to 3 mg of diol/triol in 0.75 mL of CD₂Cl₂ (used as delivered from Cambridge Isotope Laboratories). Samples were checked for chemical exchange using a standard NOESY experiment with a 1 s mixing time. For the conditions and samples used, chemical exchange would result in positive cross peaks in the spectrum (the NOE would result in negative cross peaks). Only samples which did not exhibit chemical exchange cross peaks were investigated further. The T_1 and T_2 time constants for the peaks of interest were measured for each sample as well as the translational diffusion coefficient, although we note that these constants are not critical for determining the coupling constant.

For the selective spin echo experiment, 16 spin echo times between 0.2 and 4.6 s were studied. For each of these times, 128 scans were acquired. Recycle delays greater than five times the T_1 times of the peaks of interest were used to ensure that the samples returned to equilibrium between scans. Consequently, the recycle delay times were between 18 and 23 s, resulting in total experiment times between 10 and 13 hr.

A 31 kHz RF field was used for the hard pulses. Selective pulses were between 20 ms and 40 ms in length depending on the level of selectivity required. All selective pulses were either double-selective cosine-modulated Gaussian pulses truncated at the 1% level or a regular Gaussian pulse truncated at the 1% level (for samples where the desired resonances were adjacent in the spectrum). 1 ms half-sine bell shaped gradient pulses with a maximum amplitude of 20 G cm⁻¹ were used immediately before and after the 180° selective pulse to help ensure the selection of the correct coherence transfer pathway.

A z -filter¹ was used at the end of the sequence to purge antiphase coherences; this ensured that the observed signal was pure phase. For the z -filter, a 2.3 G cm⁻¹ rectangular gradient pulse was applied synchronously with an adiabatic 180° CHIRP pulse². The CHIRP pulse was 50 ms long and the frequency of the pulse was swept through 20 kHz during this interval. This was followed by a 2 ms homospoil gradient pulse with an amplitude of 29 G cm⁻¹.

The Bruker format pulse sequence for the selective spin echo experiment is provided on the following page.

The integrals of the –OH resonances were fit to the following function using the built-in non-linear equation solver function in Excel (Microsoft Corporation, Redmond, WA).

$$S = S_0 \exp\left(-\frac{t}{T}\right) \cos(\pi Jt)$$

In this equation, t is the length of the spin-echo and S is the peak integral. The initial ($t = 0$) peak integral (S_0), the decay constant (T) and the scalar coupling constant (J) were all allowed to vary independently during the fitting process.

¹Thrippleton, M. J.; Keeler, J. *Angew. Chem., Int. Ed. Engl.* 2003, **42**, 3938–3941.

²Böhlen, J.-M.; Bodenhausen, G. *J. Magn. Reson. Ser. A.* 1993, **102**, 293–301.

```

;selse
;avance-version (loening, 06/06/12)
;1D selective spin echo
; -using selective excitation and refocussing
; -includes zero-quantum filter

#include <Avance.incl>
#include <Grad.incl>

"d12=p12*2/3.14159"
"d14=d4*0.5-(d16+p16+3u)-0.5*p12-d12"
"in14=in4*0.5"

1 ze
2 20u BLKGRAD
3 d1
  20u p10:f1 UNBLKGRAD

  p12:sp13:f1 ph1:r ; selective 90
  d14
  3u
  p16:gpl
  d16
  p12:sp14:f1 ph2:r ; selective 180
  3u
  p16:gpl
  d16

  d14 p11:f1
  d12

  (p1 ph3):f1 ; begin z-filter
  50u p10:f1
  300u gron2
  p11:sp11:f1 ph4
  d5 gron3
  50u groff
  50u p11:f1

  (p1 ph5):f1 ; end z-filter

go=2 ph31
20u BLKGRAD
d1 mc #0 to 3 F1QF(id14)
exit

ph1= 0 0 0 0 1 1 1 1 2 2 2 2 3 3 3 3
ph2= 0 1 2 3
ph3= 0 0 0 0 1 1 1 1 2 2 2 2 3 3 3 3
ph4= 0
ph5= 0
ph31=0 2 0 2 2 0 2 0

;p10 : 120dB
;p11 : f1 channel - power level for pulse (default)
;sp11: f1 channel - adiabatic inversion pulse power
;sp13: f1 channel - selective 90 pulse power
;sp14: f1 channel - selective 180 pulse power
;p1 : f1 channel - 90 degree high power pulse length
;p11: f1 channel - adiabatic inversion pulse length
;p12: f1 channel - selective 90/180 pulse length
;p16: homospoil/gradient pulse length [1 msec]
;d1 : relaxation delay; 1-5 * T1
;d4 : length of first spin echo
;d5 : homospoil after swept z-filter
;in4 : increment for the spin-echo period
;in14 : increment for each half of spin-echo period
;d16: delay for homospoil/gradient recovery [50 usec]
;NS: 8 * n, total number of scans: NS * TD0
;DS: 4

;phcor 1 : phase difference between powers sp13 and p11
;phcor 2 : phase difference between powers sp14 and p11

;spnam11: adiabatic inversion pulse
;spnam13: selective 90 pulse
;spnam14: selective 180 pulse

;for z-only gradients:
;gpz1: 33% - gradients around selective 180 pulse
;gpz2: 4% - swept z-filter gradient
;gpz3: 50% - homospoil gradient

;use gradient files:
;gpnaml: SINE.100

```

Selective Spin Echo Dephasing Curves

The time-dependence of the in-phase and antiphase magnetization for a single spin (I) coupled to one other spin (S) during the selective spin echo experiment shown in Figure 2 (MS) can be phenomenologically described by the Bloch equations:

$\frac{d\langle I_y \rangle}{dt} = \pi J \langle 2I_x S_z \rangle - R_2 \langle I_y \rangle$	(1)
$\frac{d\langle 2I_x S_z \rangle}{dt} = -\pi J \langle I_y \rangle - R_2 \langle 2I_x S_z \rangle - R_1 \langle 2I_x S_z \rangle$	(2)

where J is the I - S coupling constant, R_1 is the longitudinal relaxation rate for S and R_2 is the transverse relaxation rate constant for I . Solving this set of differential equations using the initial conditions $\langle I_y \rangle = 1$ and $\langle 2I_x S_z \rangle = 0$ results in:

$$\langle I_y \rangle = \frac{1}{2\Lambda} \exp\left[-\frac{1}{2}t(R_1 + 2R_2 + \Lambda)\right] \{[-1 + \exp(t\Lambda)]R_1 + [1 + \exp(t\Lambda)]\Lambda\} \quad (3)$$

where $\Lambda = (R_1^2 - 4J^2\pi^2)^{1/2}$. The equation predicts oscillatory behavior as long as $2\pi|J| > R_1$; if this condition is not met then the system is over damped and $\langle I_y \rangle$ never becomes negative.

In practice, it is more practical to fit the data to an exponentially damped cosine function (Eq 1, MS); this yields identical results as Eq. 3 for J when the dephasing curve passes through zero. Although this means that we need at least a single zero-crossing in the dephasing curve to accurately estimate J , this avoids the need when using equations 1(MS) or 3 to determine the values of the relaxation rates. In any case, we only report J values for experiments where a distinct zero crossing was observed.

For cases where zero crossing were not observed in the dephasing curves, we only report the maximum coupling value consistent with our observations (for example, compounds **6** and **7**).

In the selective spin echo experiments, proton exchange results in dephasing curves that are difficult to fit and lead to incorrect J values. To help reduce the amount of proton exchange, we used dilute samples (1–5 mM) in CD_2Cl_2 and added a small quantity of neutral alumina directly to the NMR tube to absorb any residual water. To assess whether proton exchange was present, chemical exchange spectroscopy (EXSY) spectra were acquired for the samples. The lack of cross-peaks connected to the hydroxyl resonances indicated the absence of proton exchange in a sample. All results in Figure 3 (MS) are from samples that were free of proton exchange.

2. Representative 2D-COSYLR spectra for diol and triol samples.

NMR spectra were obtained for diols **1**, **3**, **4**, **5**, **7**, **8**, **9**, and triol **10** on a Bruker Avance DPX 400 MHz NMR spectrometer equipped with a 5 mm dual $^1\text{H}/^{13}\text{C}$ Z-gradient probe. Diols **2** and **6** were not subject to 2D COSYLR analysis on account of their nearly degenerate OH chemical shifts. Samples were prepared by dissolving 0.5 to 3 mg of diol/triol in 0.75 mL CD_2Cl_2 (used as delivered from Cambridge Isotope Laboratories). The samples were not degassed, and spectra were recorded at 23 °C. 1D ^1H spectra and spin-lattice (T_1) relaxation times were measured with standard pulse programs. We note that knowledge of the OH T_1 values is not critical for their detection with this 2D methodology. We simply provide the T_1 values for comparative purposes. Details for the 2D experiments are as follows:

2D COSYLR experiment.³ The standard `cosylr` pulse program was used for most measurements. For several systems, a pulsed field gradient variant of the `cosylr` experiment (`cosylrgs`)⁴ was used. Acquisition parameters and OH T_1 values are provided in the figure legend for each spectrum. To ensure the detection of OH...OH scalar cross peaks, we found it useful to run a series of `cosylr` experiments with refocusing delays of 100, 200, 300, 400, and 500 ms. The data presented here are those experiments showing the strongest off-diagonal peaks. All data sets were processed with unshifted sinusoidal (SINE, SSB=0) apodization in both dimensions prior to the Fourier transformation.

<pre> ;cosylr ;avance-version ;2D homonuclear shift correlation ;with delay period to optimize for long-range couplings ;A. Bax & R. Freeman, J. Magn. Reson. 44, 542 (1981) #include <Avance.incl> ;:"d0=3u" 1 ze 2 d1 3 p1 ph1 d0 d6 p1 ph2 d6 go=2 ph31 dl wr #0 if #0 id0 zd lo to 3 times tdl exit ph1=0 0 0 0 1 1 1 1 1 2 2 2 2 3 3 3 3 ph2=0 1 2 3 ph31=0 2 0 2 3 1 3 1 2 0 2 0 1 3 1 3 ;p11 : f1 channel - power level for pulse (default) ;p1 : f1 channel - 90 degree high power pulse ;d0 : incremented delay (2D) [3 usec] ;d1 : relaxation delay; 1-5 * T1 ;d6 : delay for evolution of long range couplings ;in0: 1/(1 * SW) = 2 * DW ;nd0: 1 ;NS: 4 * n ;DS: 16 ;tdl: number of experiments ;MC2: QF </pre>	<pre> ;cosylrgs ;avance-version ;2D homonuclear shift correlation ;using gradient pulses for selection ;oleary 06/06/06 ;Lee, S-G Bulletin of the Korean Chemical Society, 22(8), 789-790. #include <Avance.incl> #include <Grad.incl> ;:"d0=3u" ;:"d13=3u" 1 ze 2 d1 3 p1 ph1 d0 d6 50u UNBLKGRAD GRADIENT(cnst21) p0 ph2 d6 GRADIENT(cnst22) d16 4u BLKGRAD go=2 ph31 dl wr #0 if #0 id0 zd lo to 3 times tdl exit ph1=0 2 ph2=0 0 2 2 ph31=0 2 ;p11 : f1 channel - power level for pulse (default) ;p0 : f1 channel - 20 to 90 degree high power pulse ;p1 : f1 channel - 90 degree high power pulse ;p16: homospoil/gradient pulse ;d0 : incremented delay (2D) [3 usec] ;d6 : refocussing delay ;d1 : relaxation delay; 1-5 * T1 ;d13: short delay [3 usec] ;d16: delay for homospoil/gradient recovery ;in0: 1/(1 * SW) = 2 * DW ;nd0: 1 ;NS: 1 * n ;DS: 16 ;tdl: number of experiments ;MC2: QF ;use gradient program (GRDPROG) : 2sine ;use gradient ratio: cnst21 : cnst22 ; 10 : 10 </pre>
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³ Bax, A.; Freeman, R. *J. Magn. Reson.* **1981**, *44*, 542.

⁴ Lee, S.-G. *Bull. Korean Chemical Society*, **2001**, *22*, 789-790.

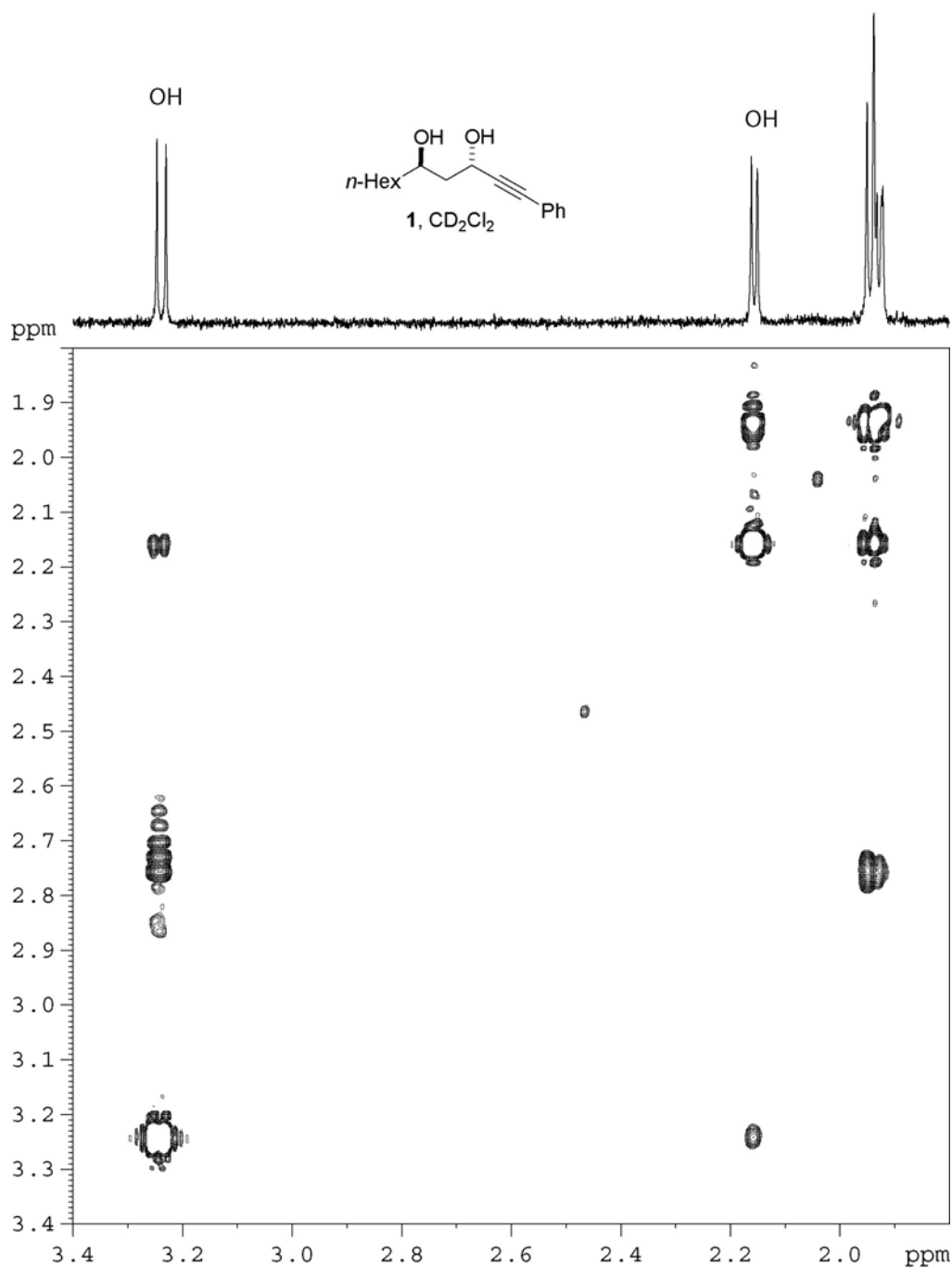


Figure S2.1. Pulse program: cosy1r. F2 and F1 sweep widths: 853.8 Hz. 128 FIDs recorded, each consisting of 32 scans and 512 data points (AQ = 0.2999 s). A refocussing delay (D6) of 400 ms and a recycle delay of (D1) of 1.5 s was employed. Zero-filling (2K x 2K) was applied to achieve digital resolution of 0.417 Hz/pt in each dimension. T_1 (OH low field) = 4.2 s, T_1 (OH high field) = 3.3 s.

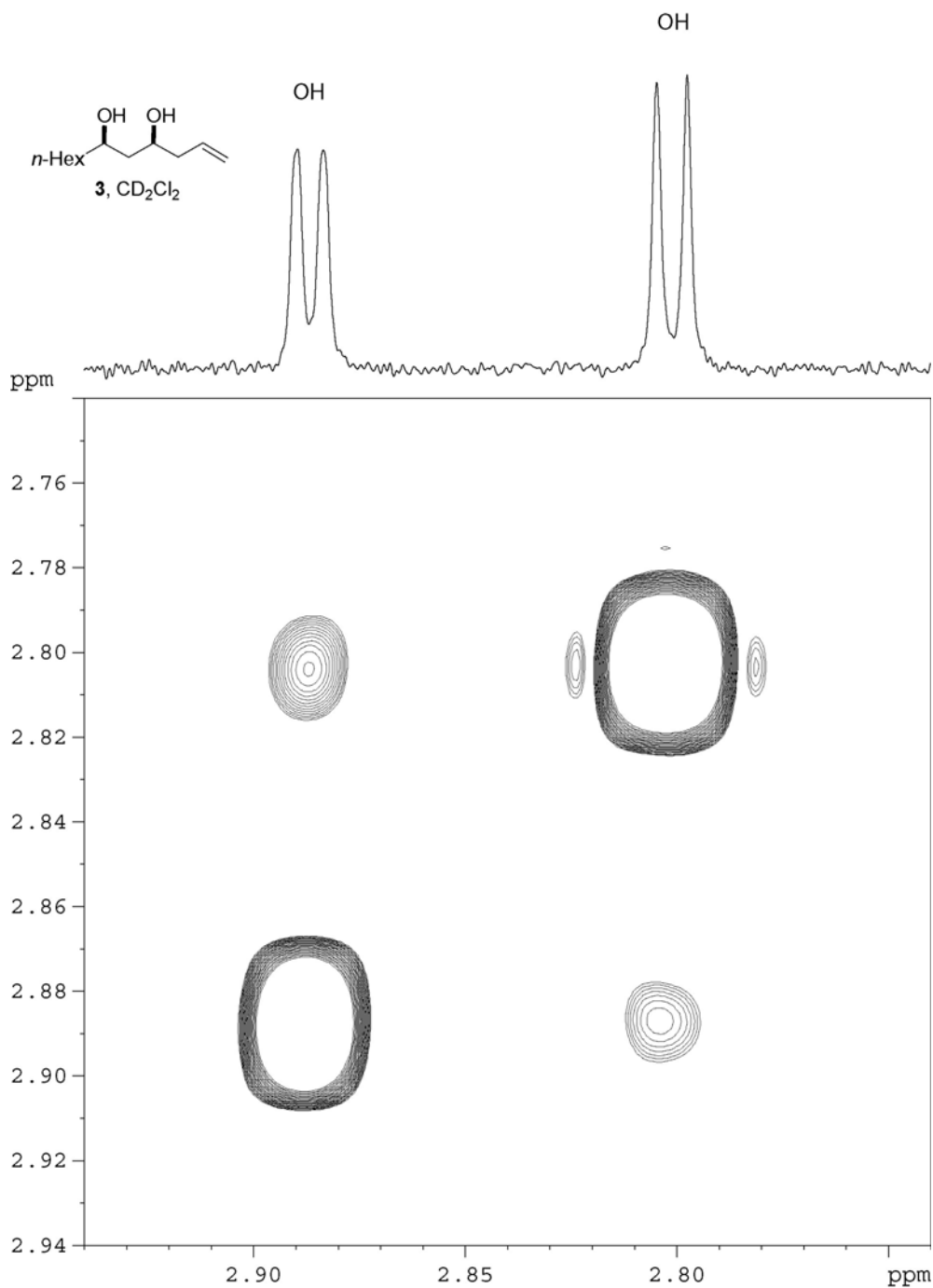


Figure S2.2. Pulse program: cosyldr. F2 and F1 sweep widths: 703.8 Hz. 128 FIDs recorded, each consisting of 8 scans and 512 data points (AQ = 0.3638 s). A refocussing delay (D6) of 300 ms and a recycle delay of (D1) of 1.5 s was employed. Zero-filling (2K x 2K) was applied to achieve digital resolution of 0.344 Hz/pt in each dimension. T_1 (OH low field) = 4.1 s, T_1 (OH high field) = 3.9 s.

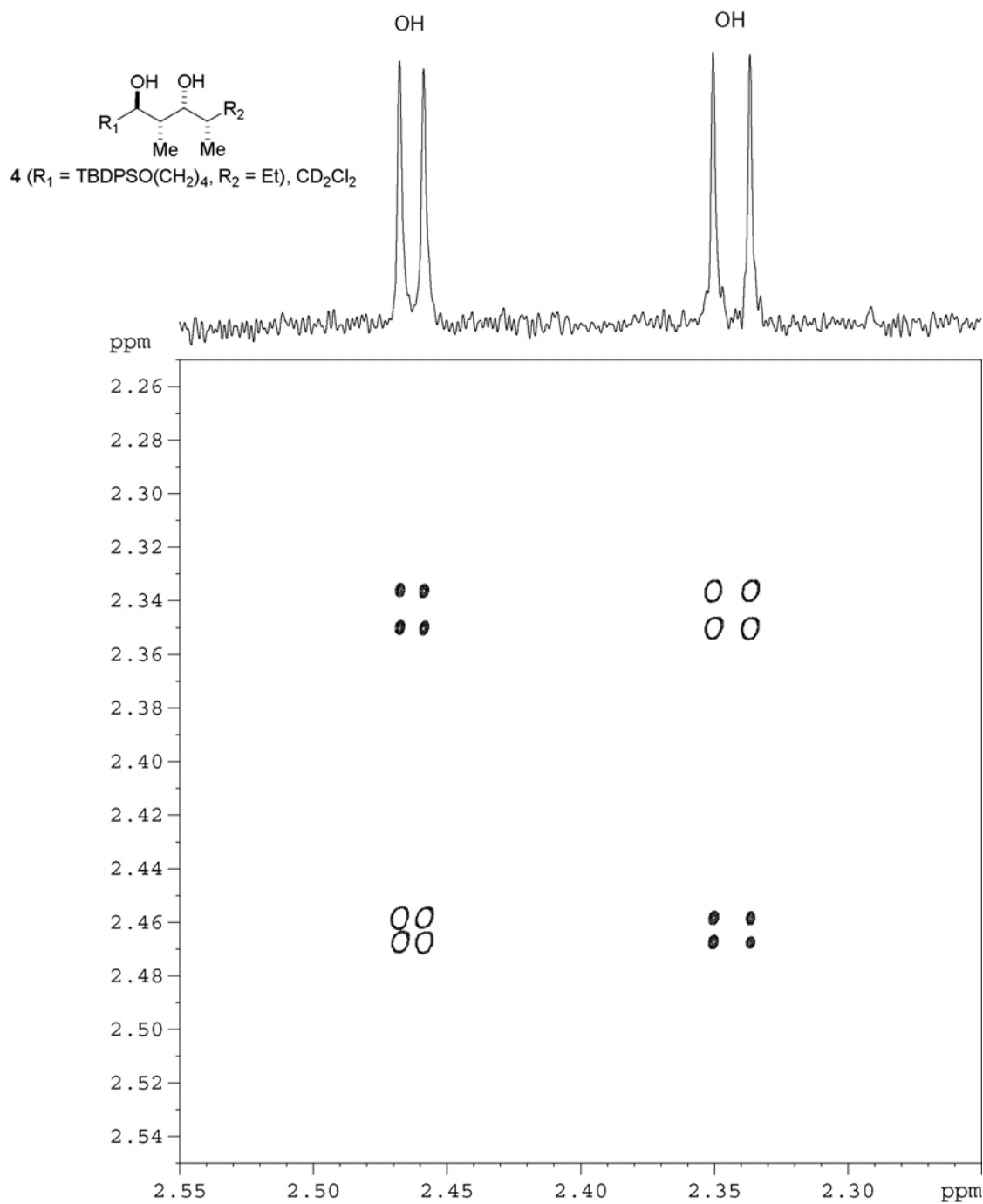


Figure S2.3. Pulse program: cosy1r. F2 and F1 sweep widths: 155.0 Hz. 128 FIDs recorded, each consisting of 8 scans and 512 data points ($AQ = 1.652$ s). A refocussing delay (D6) of 400 ms and a recycle delay of (D1) of 1.5 s was employed. Zero-filling (512W in F1) was applied to achieve digital resolution of 0.302 Hz/pt in each dimension. T_1 (OH low field) = 2.7 s, T_1 (OH high field) = 2.5 s.

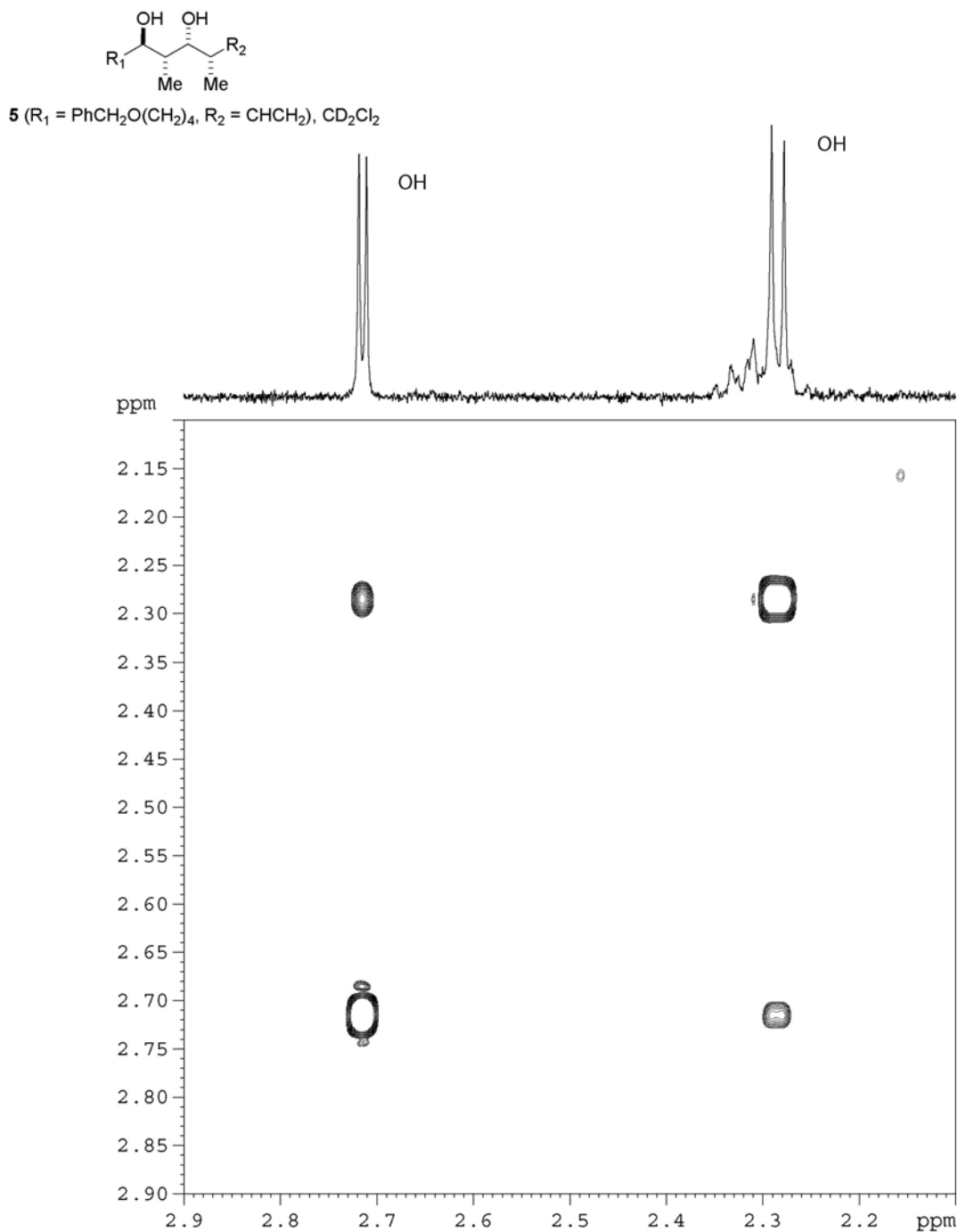


Figure S2.4. Pulse program: cosy1r. F2 and F1 sweep widths: 744.0 Hz. 128 FIDs recorded, each consisting of 32 scans and 512 data points (AQ = 0.344 s). A refocussing delay (D6) of 500 ms and a recycle delay of (D1) of 1.5 s was employed. Zero-filling (2K x 2K) was applied to achieve digital resolution of 0.363 Hz/pt in each dimension. T_1 (OH low field) = 3.5 s, T_1 (OH high field) = 3.2 s.

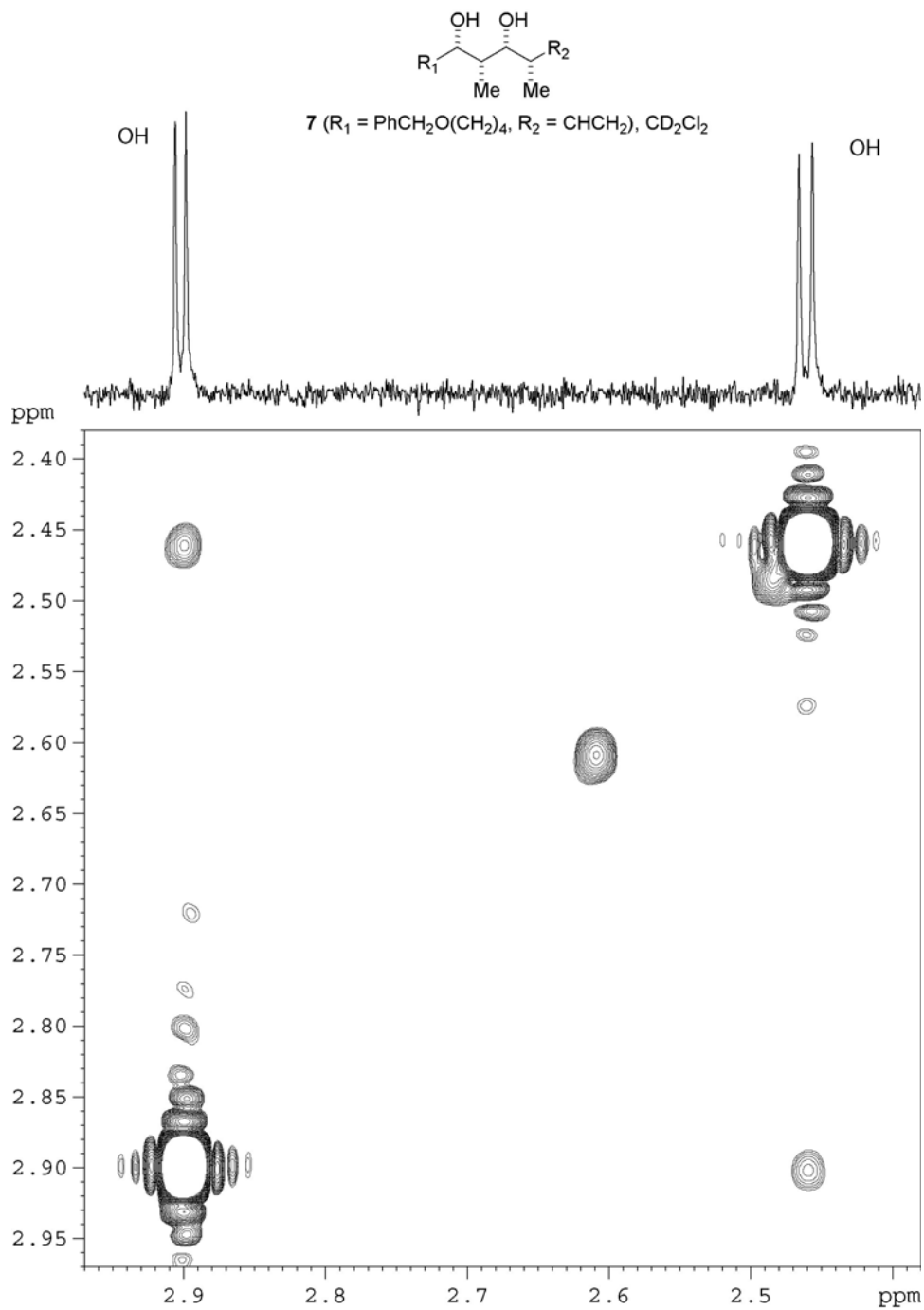


Figure S2.5. Pulse program: cosy1r. F2 and F1 sweep widths: 826.7 Hz. 128 FIDs recorded, each consisting of 32 scans and 512 data points (AQ = 0.3097 s). A refocussing delay (D6) of 200 ms and a recycle delay of (D1) of 1.5 s was employed. Zero-filling (2K x 2K) was applied to achieve digital resolution of 0.404 Hz/pt in each dimension. T_1 (OH low field) = 3.2 s, T_1 (OH high field) = 3.1 s.

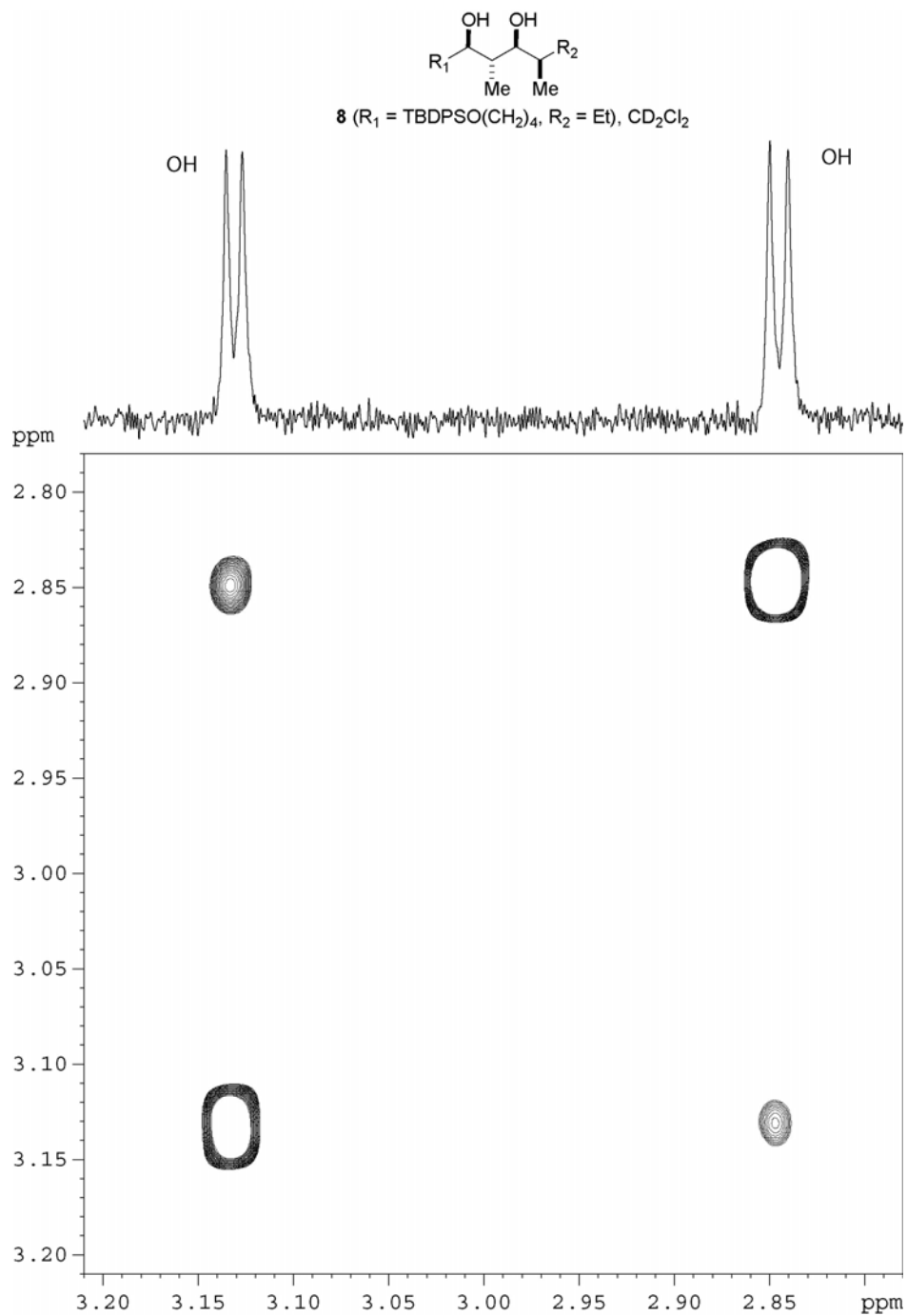


Figure S2.6. Pulse program: cosy1r. F2 and F1 sweep widths: 659.3 Hz. 128 FIDs recorded, each consisting of 8 scans and 512 data points (AQ = 0.3884 s). A refocussing delay (D6) of 400 ms and a recycle delay (D1) of 1.5 s was employed. Zero-filling (2K x 2K) was applied to achieve digital resolution of 0.322 Hz/pt in each dimension. T_1 (OH low field) = 2.3 s, T_1 (OH high field) = 2.3 s.

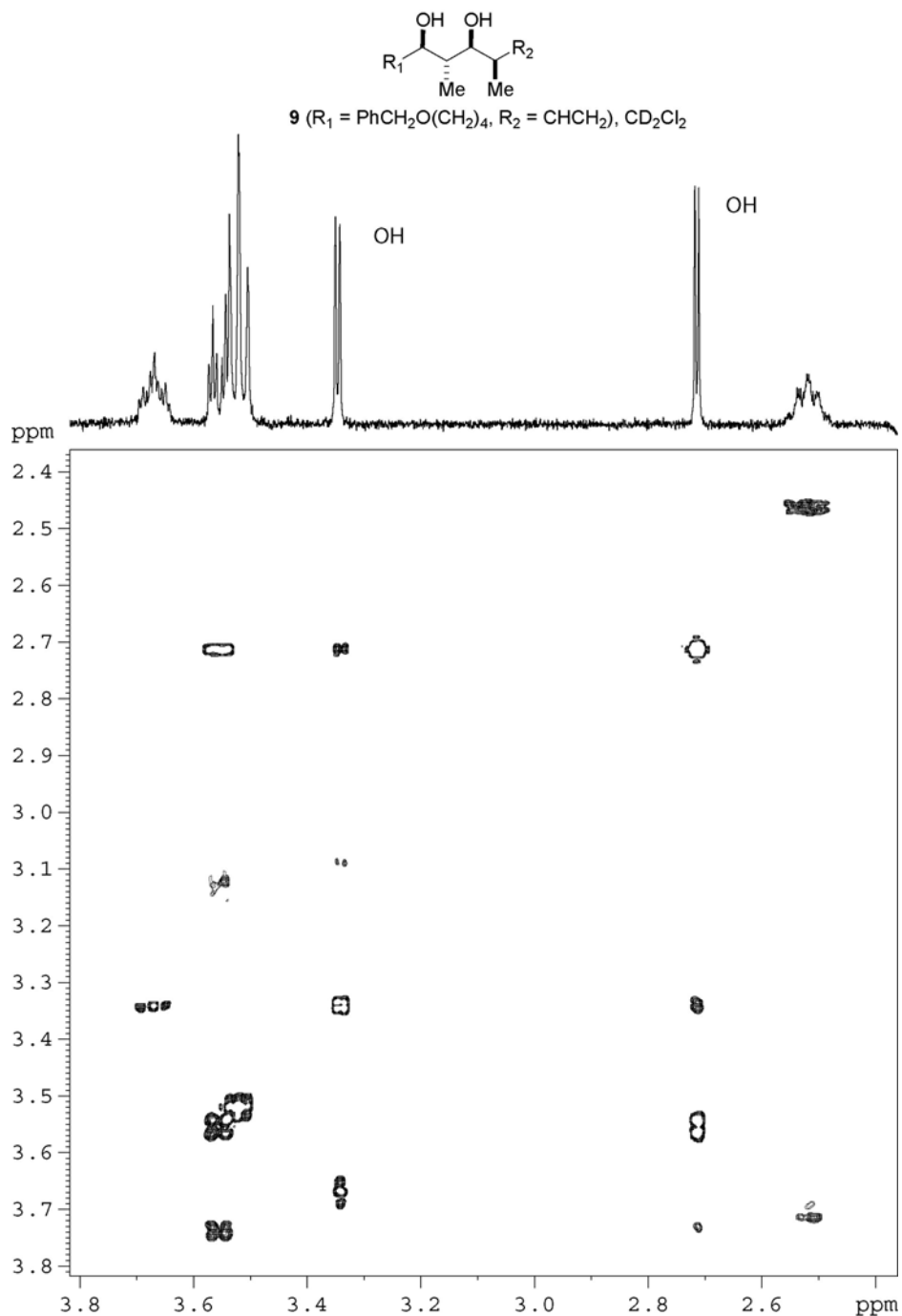


Figure S2.7. Pulse program: cosy1rgs. F2 and F1 sweep widths: 583.0 Hz. 128 FIDs recorded, each consisting of 4 scans and 512 data points (AQ = 0.439 s). A refocussing delay (D6) of 300 ms and a recycle delay of (D1) of 1.5 s was employed. Zero-filling (2K x 2K) was applied to achieve digital resolution of 0.285 Hz/pt in each dimension. T_1 (OH low field) = 2.8 s, T_1 (OH high field) = 3.1 s.

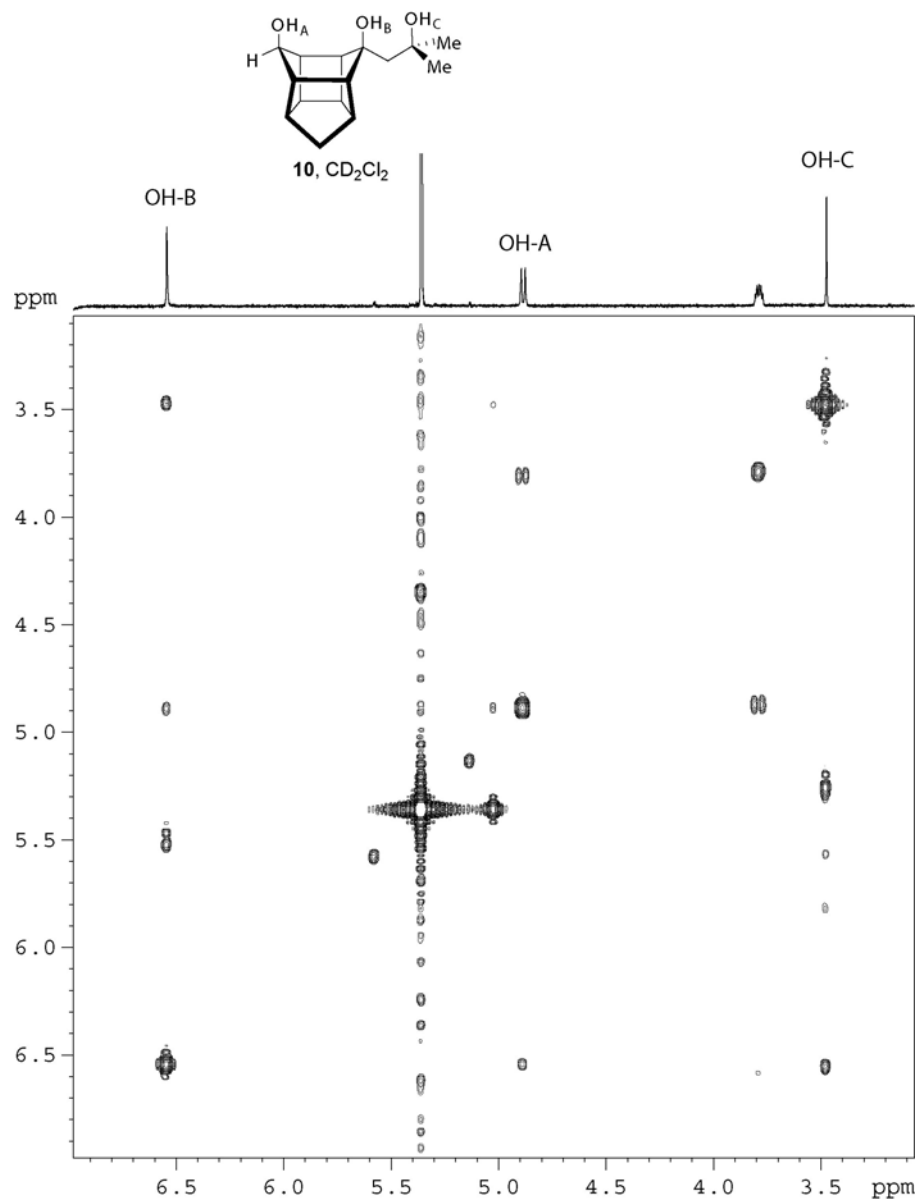


Figure S2.8. Pulse program: cosyldr. F2 and F1 sweep widths: 1566.4 Hz. 128 FIDs recorded, each consisting of 32 scans and 512 data points (AQ = 0.1635 s). A refocussing delay (D6) of 200 ms and a recycle delay of (D1) of 1.5 s was employed. Zero-filling (2K x 2K) was applied to achieve digital resolution of 0.765 Hz/pt in each dimension. T_1 (OH-B) = 3.3 s, T_1 (OH-A) = 3.1 s, T_1 (OH-C) = 3.6 s.

3. Computational studies of syn- and anti-2,4-pentanediol.

Conformer Identification & Geometry Optimization

The conformer energies of syn- and anti-2,4-pentanediol were surveyed using MP2/6-31G* theory with the conformer distribution subroutine in Spartan '04.⁵ Coordinates for conformers whose relative energies ranged from 0 to 10 kcal/mol were transferred to Gaussian 03W⁶ and further studied with a variety of approaches.

We found the conformer relative energies were very dependent upon the type and level of theory. This behavior for two syn conformers is illustrated in **Table S3.1**. Clearly, relative energies in systems such as these should be interpreted with caution.

Not surprisingly, we also found that the conformer relative energies changed when the calculations included a polarizable continuum model (PCM) for CH₂Cl₂ (the solvent used for the NMR experiments). When calculations are performed in the gas phase, both *syn*- and *anti*-2,4-pentanediol are predicted to exist nearly exclusively in conformations containing intramolecular hydrogen bonds (**Tables S3.2 & S3.3**). When PCM is used, the anti isomer was shown to exist ca. 33% in non-hydrogen-bonded conformations. On the other hand, the syn isomer retains a strong preference (ca. 94%) for H-bonded conformations. Additionally, the PCM calculations suggest the anti stereoisomer is conformationally more diverse (11 conformers found) than the syn isomer (4 conformers found, but only two account for 94% of the population).

A recent paper examined the preferred backbone conformation of *syn*- and *anti*-2,4-pentanediol.⁷ The hydroxyl orientations were not explicitly considered in this paper. It is also unclear how the authors explored the pentanediol conformational space, as only staggered conformations are considered. Their computational study was done in the gas phase, which was appropriate because comparisons were being made with matrix isolation IR experiments. We find that partially eclipsed 'twist' conformations (e.g. *anti*-91 and *anti*-92, **Table S3.2**) are predicted to contribute to the conformer population when either gas-phase or PCM (CH₂Cl₂) model chemistry is employed. It therefore seems unlikely that only fully staggered conformations are the only contributing structures in this system.

In the work presented here, we decided to systematically compare the pentanediol conformers energies at the MP2/6-311G(d,p) level of theory. Our choice of this model chemistry

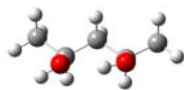
⁵ Spartan '04, Wavefunction, Inc., Irvine, CA.

⁶ Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

⁷ Manzanares, C. E.; Reynolds, D.; Lewis, E. K.; Moehnke, C. J.; Mina-Camilde, N.; Salazar, M. C.; Hernandez, A. *J. J. Mol. Structure*, **204**, 689, 183-190.

does not imply that we feel it is uniquely correct, but rather, that it provides a reasonable picture of the system under study.

Table S3.1. Gas-phase syn-2,4-pentanediol conformer populations computed with various types and levels of theory.



Conformer 001 TT(TG+)



Conformer 023 TT(G-G-)

conformer	model chemistry/population (two conformer Boltzmann weighting)
	B3LYP/6-31G* (E)
TT(TG+) 001	28.76
TT(G-G-) 023	71.24
	MP2/6-31G* (E)
TT(TG+) 001	40.14
TT(G-G-) 023	59.86
	B3LYP/6-31G** (E)
TT(TG+) 001	30.18
TT(G-G-) 023	69.82
	MP2/6-31G** (E)
TT(TG+) 001	39.61
TT(G-G-) 023	60.39
	B3LYP/6-31+G** (E)
TT(TG+) 001	57.31
TT(G-G-) 023	42.69
	MP2/6-31+G** (E)
TT(TG+) 001	67.23
TT(G-G-) 023	32.77
	B3LYP/6-311G** (E)
TT(TG+) 001	41.70
TT(G-G-) 023	58.30
	MP2/6-311G** (E)
TT(TG+) 001	48.0
TT(G-G-) 023	52.0
	B3LYP/6-311+G** (E)
TT(TG+) 001	62.37
TT(G-G-) 023	37.63
	MP2/6-311+G** (E)
TT(TG+) 001	73.10
TT(G-G-) 023	26.90

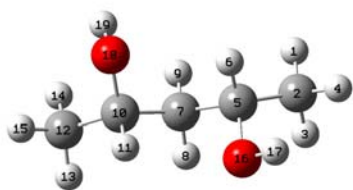
Table S3.2. Anti-2,4-pentanediol conformational energies. Blue: conformer with intramolecular H-bond. Red: conformer without intramolecular H-bond.

theory / file name	6	7	7a	8	9a	13	15	15a	23	31	91	92
conformer identity in manuscript	12e	12b					12a		12c	12d		
mp2/6-311G**/opt (Energy, Hartrees)	-347.4361294	-347.4390303	-347.4363502	-347.4355724	-347.4339552	-347.4335596	-347.4386434	-347.4339912	-347.4391258	-347.4388274	-347.4381217	-347.4382694
PCM (CH2Cl2) mp2/6-311G** opt (Energy, Hartrees)	-347.4499958	-347.4503809	-347.4497287	-347.4499315	-347.4472994	-347.4473433	-347.4496725	-347.4442407	-347.4504268	-347.4495413	-347.4494765	-347.4495093
mp2/6-311G**/opt (relative energy, kcal/mol)	1.8802695	0.0599272	1.7417154	2.2297923	3.2446006	3.4928434	0.3027106	3.2220103	0.0000000	0.1872488	0.6300823	0.5373991
PCM (CH2Cl2) mp2/6-311G** opt (relative E, kcal/mol)	0.2704566	0.0288027	0.4380644	0.3108055	1.9624732	1.9349255	0.4733304	3.8818365	0.0000000	0.5556597	0.5963223	0.5757400
Population analysis based upon deIE (gas phase):												
Nj	0.0418553	0.9038014	0.0528824	0.0232032	0.0041849	0.0027525	0.5999446	0.0043476	1.0000000	0.7290299	0.3452594	0.4037224
Nj/N (Boltzmann population)	0.0101813	0.2198504	0.0128637	0.0056442	0.0010180	0.0006695	0.1459370	0.0010575	0.2432508	0.1773371	0.0839846	0.0982058
N	4.1109834											
Gas Phase non-H-bond vs. H-bond%	0.0303767	0.9696233										
Population analysis based upon deIE (CH2Cl2 PCM):												
Nj	0.6335101	0.9525492	0.4774148	0.5918035	0.0364329	0.0381669	0.4498271	0.0014275	1.0000000	0.3914694	0.3655037	0.3784241
Nj/N (Boltzmann population)	0.1191586	0.1791675	0.0897982	0.1113139	0.0068528	0.0071789	0.0846092	0.0002685	0.1880926	0.0736325	0.0687486	0.0711788
N	5.3165293											
PCM(CH2Cl2) non-H-bond vs. H-bond%	0.3343023	0.6656977										

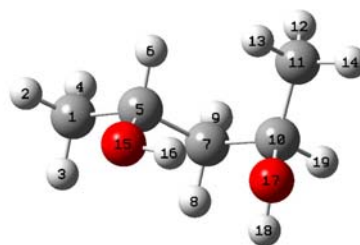
Table S3.3 Syn-2,4-pentanediol conformational energies. Blue: conformer with intramolecular H-bond. Red: conformer without H-bond.

file name	1	3	23	34	45	71
conformer identity in manuscript	11a		11b			
mp2/6-311G**/opt (Energy, Hartrees)	-347.4400630	-347.4364373	-347.4401306	-347.4361371	-347.4349018	-347.4347751
mp2/6-311G**/solvent opt (Energy, Hartrees)	-347.4515626	-347.4469689	-347.4509828	-347.4465804	-347.4486296	-347.4484200
mp2/6-311G**/opt (relative E, kcal/mol)	0.0424196	2.3175808	0.0000000	2.5059592	3.2811217	3.3606271
mp2/6-311G**/solvent opt (relative E, kcal/mol)	0.0000000	2.8825904	0.3638300	3.1263778	1.8404854	1.9720114
Population analysis based upon ΔE (gas phase)						
N _j	0.9309066	0.0200077	1.0000000	0.0145585	0.0039347	0.0034406
N _j /N (Boltzmann population)	0.4718592	0.0101415	0.5068814	0.0073794	0.0019944	0.0017440
N	1.9728482					
H-bond vs non-H-bond %		0.9962615			0.0037384	
Population analysis based upon ΔE (PCM CH ₂ Cl ₂)						
N _j	1.0000000	0.0077098	0.5411407	0.0051091	0.0447623	0.0358511
N _j /N (Boltzmann population)	0.6117806	0.0047167	0.3310594	0.0031256	0.0273847	0.0219330
N	1.6345729					
H-bond vs non-H-bond %		0.9506823			0.0493177	

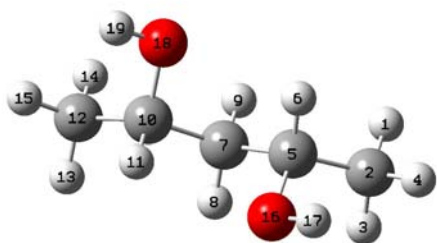
Figure S3.1. Anti-2,4-pentanediol conformers and filename/manuscript number identification.



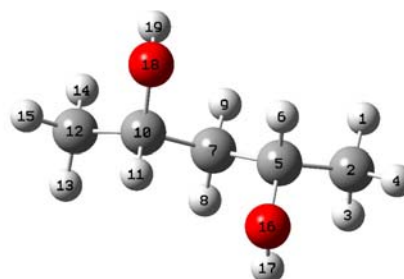
Filename: 6, manuscript: **12e**



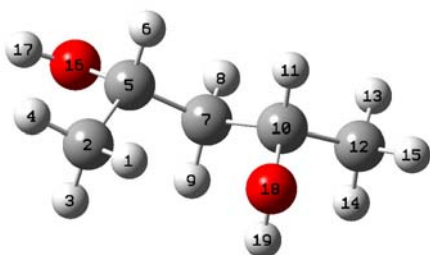
Filename: 7, manuscript: **12b**



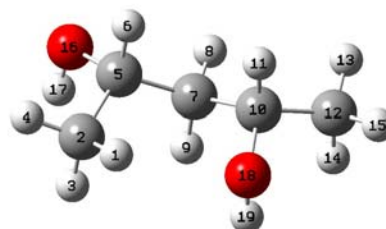
Filename: 7a



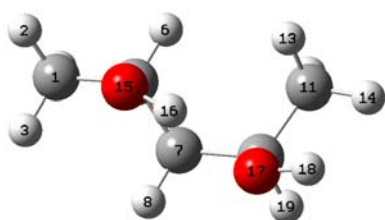
Filename: 8



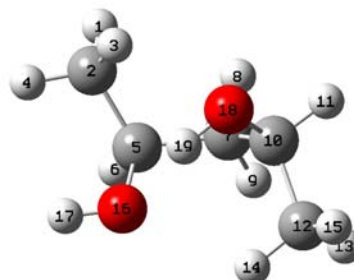
Filename: 9a



Filename: 13

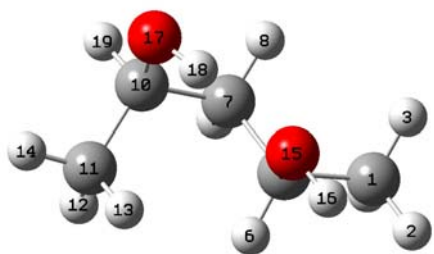


Filename: 15, manuscript: **12a**

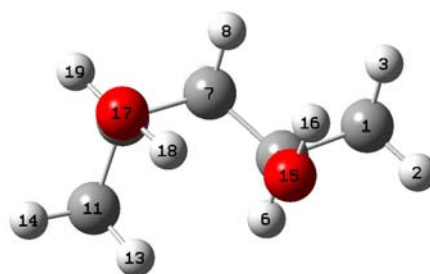


Filename: 15a

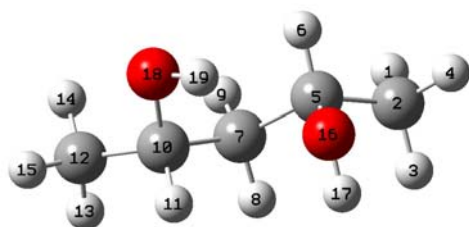
Figure S3.1. Anti-2,4-pentanediol conformers and filename/manuscript number identification (cont.).



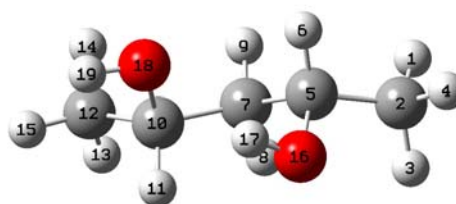
Filename: 23, manuscript: **12c**



Filename: 31, manuscript: **12d**

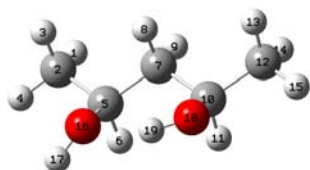


Filename: 91

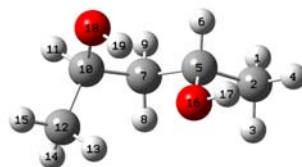


Filename: 92

Figure S3.2. Syn-2,4-pentandiol conformers and filename/manuscript number identification.



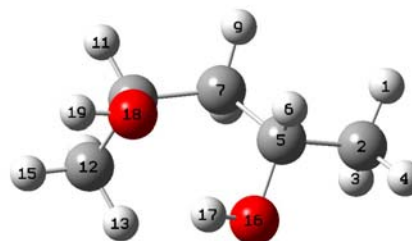
Filename: 1, manuscript: **11a**



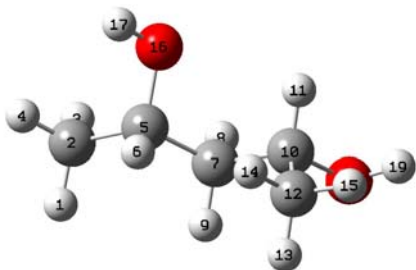
Filename: 3



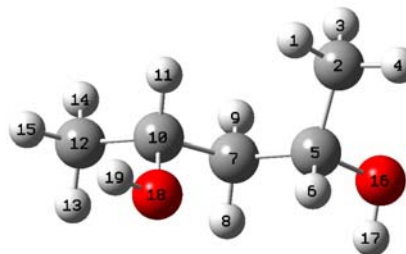
Filename: 23, manuscript: **11b**



Filename: 34



Filename: 71



Filename: 45

Calculation of OH \cdots OH Coupling Constants

Syn- and *anti*-2,4-pentanediol MP2 geometries were used for DFT UB3PW91/6-311G(d,p) NMR calculations, which were performed three different ways. In the first approach, a gas-phase NMR calculation was performed using the gas-phase optimized geometry. We also performed a PCM NMR calculation using the gas-phase geometry and a PCM NMR calculation using the PCM-optimized geometry. The results are compiled in **Tables S3.4** and **S3.5**. Any variability between the all-gas-phase calculations and those using a PCM-NMR calculation on the gas-phase structures must only be due to the inclusion/omission of PCM in the NMR calculation, as the molecular geometries are identical for each set of calculations. The inclusion of PCM in the NMR calculation can account for up to ca. 50% variability in the computed J (**Table S3.4**). In the manuscript, we only report J values computed with PCM in both the optimization and NMR calculation. Our reason for doing this is based upon the notion that PCM-corrected NMR parameters are usually in better agreement with experimental data.⁸

For each conformer, **Tables S3.4** and **S3.5** tabulate the Fermi contact contribution to J (J_{FC}) and J_{tot} , which consists of contributions from the Fermi contact (FC) term, the spin dipolar (SD) term, the paramagnetic spin-orbital (PSO) term, and the diamagnetic spin-orbital (DSO) term. The FC contribution can be negative or positive, and it can be small for certain OH \cdots OH intramolecular hydrogen bond orientations (e.g., *syn*-3, **Table S3.5**) as well as in conformations lacking intramolecular hydrogen bonds (*syn*-71, **Table S3.5**). In each table, we also include a Boltzmann-weighted J_{FC} and J_{tot} calculation, using the PCM-MP2/6-311G(d,p) energies. As mentioned earlier, the basis set-dependence of the energies precludes a rigorous interpretation of these population-averaged values.

We noticed that certain calculations produced small J_{FC} terms in conformations that gave reasonably large J_{tot} values. This was particularly evident in conformations lacking intramolecular hydrogen bonds (see: *syn*-71 in **Table S3.5**). If this were the case, then it would suggest an alternate long-range coupling mechanism, i.e., one not involving hydrogen bond-mediated transmission. We suspected that these effects were due to the use of insufficient basis sets, and so we explored the spin-spin coupling with larger basis sets for two *syn* conformers—one with an intramolecular hydrogen bond (*syn*-1) and one without (*syn*-71).

Closed shell calculations (these give the same results as open shell⁹) were used to investigate the basis set dependencies of the OH \cdots OH coupling constants. The results for increasingly larger basis sets, which are given in **Table S3.6**, are computationally intensive: the largest job that we were able to complete successfully (rb3pw91/cc-pVQZ for *syn*-1) required five days using a 3.6 GHz single processor Pentium 4 workstation.

As shown in **Table S3.6**, when higher levels of theory were employed, the FC term remained relatively constant for either conformer. In the conformation lacking the intramolecular hydrogen bond (*syn*-71), the J_{tot} term was observed to diminish with increasing bases. In the highest-level calculation of *syn*-71 (rb3pw91/cc-pVQZ), $J_{\text{tot}} = -0.02$ Hz, which supports our contention that the hydrogen bond is important for mediating the spin-spin coupling in these systems. Indeed, for the isomer with an intramolecular hydrogen bond (*syn*-1) both J_{FC} and J_{tot} are reasonably large (-0.60 to -0.79 Hz) and constant with increasing basis sets. These calculations also show that the percentage of the total coupling due to the Fermi contact term

⁸ Miertus S, Scrocco E, Tomasi J, *Chem. Phys.* **1981**, *55*, 117-129.

⁹ Salvador, P.; Dannenberg, J. J. *J. Phys. Chem. B* **2004**, *108*, 15370-15375.

increases ($J_{\text{FC}}/J_{\text{tot}} = 0.80$ for rb3pw91/cc-pVTZ, $J_{\text{FC}}/J_{\text{tot}} = 0.97$ for rb3pw91/cc-pVQZ) with the use of larger basis sets in the calculation.

Table S3.4 Anti-2,4-pentanediol NMR calculations. Blue: conformer with intramolecular H-bond. Red: conformer without intramolecular H-bond.

theory / file name:	6	7	7a	8	9a	13	15	15a	23	31	91	92
conformer identity in manuscript:	12e	12b					12a		12c	12d		
OH proton labels:	19-17	16-18	19-17	19-17	19-17	19-17	16-18	19-17	16-18	16-18	19-17	19-17
mp2/6-311G**//ub3pw91/6-311G** J(FC), Hz	0.004	0.234	-0.023	-0.004	0.003	-0.001	-0.481	-0.073	-0.805	0.189	-0.111	0.010
mp2/6-311G**//ub3pw91/6-311G** J(total), Hz	-0.288	0.421	-0.286	-0.302	-0.208	-0.058	-0.540	-0.035	-1.002	0.487	-0.247	0.047
PCM/mp2/6-311G**//ub3pw91/6-311G** J(FC), Hz	-0.001	0.228	-0.015	-0.003	0.007	-0.002	-0.711	-0.184	-0.605	0.175	-0.009	0.029
PCM/mp2/6-311G**//ub3pw91/6-311G** J(total), Hz	-0.276	0.390	-0.241	-0.298	-0.209	-0.056	-0.798	-0.170	-0.714	0.512	-0.152	0.097
PCM/mp2/6-311G**//PCM/ub3pw91/6-311G** J(FC), Hz	-0.002	0.215	-0.014	-0.003	0.007	-0.002	-0.659	-0.183	-0.571	0.163	-0.008	0.025
PCM/mp2/6-311G**//PCM/ub3pw91/6-311G** J(total), Hz	-0.281	0.368	-0.243	-0.301	-0.212	-0.058	-0.744	-0.169	-0.679	0.498	-0.153	0.090
gas phase O-O distance (Å)	3.583	2.802	3.523	3.623	4.419	4.473	2.762	2.775	2.768	2.815	2.917	2.893
Boltzmann-weighted J(OH/OH) Hz												
mp2/6-311G**//ub3pw91/6-311G** J(FC), Hz	-0.190											
mp2/6-311G**//ub3pw91/6-311G** J(total), Hz	-0.168											
PCM/mp2/6-311G**//ub3pw91/6-311G** J(FC), Hz	-0.121											
PCM/mp2/6-311G**//ub3pw91/6-311G** J(total), Hz	-0.187											
PCM/mp2/6-311G**//PCM/ub3pw91/6-311G** J(FC), Hz	-0.113											
PCM/mp2/6-311G**//PCM/ub3pw91/6-311G** J(total), Hz	-0.183											

Table S3.5 Syn-2,4-pentanediol NMR calculations. Blue: conformer with intramolecular H-bond. Red: conformer without intramolecular H-bond.

theory / file name:	1	3	23	34	45	71
conformer identity in manuscript:	11a		11b			
OH proton labels:	17-19	17-19	17-19	17-19	17-19	17-19
mp2/6-311G**//ub3pw91/6-311G** FC	-0.654	-0.022	0.223	-0.019	0.001	0.037
mp2/6-311G**//ub3pw91/6-311G** total J	-0.792	0.008	0.427	0.026	-0.253	-0.231
PCM/mp2/6-311G**//ub3pw91/6-311G** FC	-0.353	0.097	0.222	-0.114	0.005	0.067
PCM/mp2/6-311G**//ub3pw91/6-311G** total J	-0.379	0.228	0.468	-0.110	-0.246	-0.188
PCM/mp2/6-311G**//PCM/ub3pw91/6-311G** FC	-0.318	0.083	0.208	-0.111	0.006	0.064
PCM/mp2/6-311G**//PCM/ub3pw91/6-311G** total J	-0.352	0.209	0.448	-0.108	-0.246	-0.193
Gas phase O---O distance (Å)	2.750	2.829	2.792	2.798	4.171	4.130
Boltzmann-weighted J(OH/OH) Hz						
mp2/6-311G**//ub3pw91/6-311G** FC	-0.196					
mp2/6-311G**//ub3pw91/6-311G** total J	-0.158					
PCM/mp2/6-311G**//ub3pw91/6-311G** FC	-0.141					
PCM/mp2/6-311G**//ub3pw91/6-311G** total J	-0.087					
PCM/mp2/6-311G**//PCM/ub3pw91/6-311G** FC	-0.124					
PCM/mp2/6-311G**//PCM/ub3pw91/6-311G** total J	-0.077					

Table S3.6 Syn-2,4-pentanediol NMR J calculations (Hz) at increasing levels of theory for the NMR calculation on a fixed diol geometry. Blue: conformer with intramolecular H-bond. Red: conformer without intramolecular H-bond.

theory / file name:	1		71
conformer identity in manuscript:	11a		
OH proton labels:	17-19		17-19
mp2/6-311G**//ub3pw91/6-311G** FC	-0.65	b3lyp/6-311G**//ub3pw91/6-311G** FC	0.05
mp2/6-311G**//ub3pw91/6-311G** total J	-0.79	b3lyp/6-311G**//ub3pw91/6-311G** total J	-0.22
mp2/6-311G**//rb3pw91/6-311G** FC	-0.65	b3lyp/6-311G**//rb3pw91/6-311G** FC	0.05
mp2/6-311G**//rb3pw91/6-311G** total J	-0.79	b3lyp/6-311G**//rb3pw91/6-311G** total J	-0.22
mp2/6-311G**//rb3pw91/cc-pVTZ FC	-0.60	b3lyp/6-311G**//rb3pw91/cc-pVTZ FC	0.04
mp2/6-311G**//rb3pw91/cc-pVTZ total J	-0.75	b3lyp/6-311G**//rb3pw91/cc-pVTZ total J	-0.16
mp2/6-311G**//rb3pw91/cc-pVQZ FC	-0.65	b3lyp/6-311G**//rb3pw91/cc-pVQZ FC	0.05
mp2/6-311G**//rb3pw91/cc-pVQZ total J	-0.67	b3lyp/6-311G**//rb3pw91/cc-pVQZ total J	-0.02
Gas phase O---O distance (Å)	2.750		4.130

Table 3.7. Optimized Cartesian coordinates for anti isomer 6. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.329188	1.403529	1.277601
2	6	0	2.470849	0.749720	0.411660
3	1	0	2.646530	1.364502	-0.475454
4	1	0	3.363534	0.141116	0.589717
5	6	0	1.252557	-0.134354	0.190116
6	1	0	1.064356	-0.743305	1.084048
7	6	0	-0.002459	0.669791	-0.099344
8	1	0	0.133582	1.183855	-1.058834
9	1	0	-0.132643	1.437130	0.676291
10	6	0	-1.253723	-0.200473	-0.148606
11	1	0	-1.065501	-1.030983	-0.832299
12	6	0	-2.477761	0.580124	-0.602338
13	1	0	-2.340517	0.975191	-1.612901
14	1	0	-2.657945	1.425805	0.072282
15	1	0	-3.359455	-0.064662	-0.589401
16	8	0	1.439659	-0.979937	-0.945296
17	1	0	2.162685	-1.573575	-0.730340
18	8	0	-1.486620	-0.820266	1.116365
19	1	0	-1.704910	-0.105831	1.721817

Table 3.8. Optimized Cartesian coordinates for anti isomer 6. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.309239	1.382880	1.315518
2	6	0	2.461917	0.756669	0.431002
3	1	0	2.626815	1.401459	-0.437327
4	1	0	3.361823	0.153793	0.588676
5	6	0	1.255679	-0.138372	0.184082
6	1	0	1.077273	-0.769862	1.065410
7	6	0	-0.004808	0.666316	-0.082730
8	1	0	0.127546	1.209755	-1.027552
9	1	0	-0.136843	1.411364	0.714399
10	6	0	-1.259484	-0.195871	-0.159307
11	1	0	-1.084039	-0.996966	-0.883817
12	6	0	-2.479987	0.612724	-0.574733
13	1	0	-2.339519	1.051419	-1.567064
14	1	0	-2.653409	1.426080	0.139458
15	1	0	-3.366669	-0.025963	-0.592039
16	8	0	1.458491	-0.958498	-0.967670
17	1	0	2.127204	-1.620722	-0.730848
18	8	0	-1.490594	-0.872318	1.077176
19	1	0	-1.632507	-0.185509	1.749257

Table 3.9. Optimized Cartesian coordinates for anti isomer 7. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.536114	-0.446443	0.129197
2	1	0	-3.220223	-0.128846	-0.661124
3	1	0	-2.773662	0.115439	1.036874
4	1	0	-2.683973	-1.513483	0.318679
5	6	0	-1.105736	-0.161263	-0.290919
6	1	0	-0.878990	-0.769890	-1.179585
7	6	0	-0.113633	-0.522697	0.812505
8	1	0	-0.374662	0.057336	1.708477
9	1	0	-0.232042	-1.583512	1.067280
10	6	0	1.357036	-0.268564	0.473232
11	6	0	1.816564	-0.944495	-0.805032
12	1	0	1.600584	-2.015632	-0.772347
13	1	0	1.309135	-0.508749	-1.668810
14	1	0	2.891569	-0.802492	-0.934392
15	8	0	-1.039806	1.219518	-0.619280
16	1	0	-0.103368	1.448944	-0.602969
17	8	0	1.610362	1.134405	0.286745
18	1	0	1.421758	1.564489	1.126134
19	1	0	1.970719	-0.634228	1.308168

Table 3.10. Optimized Cartesian coordinates for anti isomer 7. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.539698	-0.432891	0.131158
2	1	0	-3.224620	-0.115892	-0.659874
3	1	0	-2.771294	0.133291	1.038174
4	1	0	-2.695634	-1.497940	0.325390
5	6	0	-1.106157	-0.165127	-0.290180
6	1	0	-0.886846	-0.778458	-1.177312
7	6	0	-0.117546	-0.525761	0.814779
8	1	0	-0.374887	0.055089	1.711178
9	1	0	-0.236236	-1.587603	1.065906
10	6	0	1.352520	-0.267938	0.473650
11	6	0	1.809155	-0.953716	-0.801041
12	1	0	1.584391	-2.023141	-0.764970
13	1	0	1.306119	-0.517677	-1.668064
14	1	0	2.886024	-0.822089	-0.929893
15	8	0	-1.016274	1.217419	-0.633402
16	1	0	-0.082732	1.446200	-0.524275
17	8	0	1.594992	1.137094	0.277657
18	1	0	1.508630	1.568069	1.147210
19	1	0	1.967696	-0.623351	1.312293

Table 3.11. Optimized Cartesian coordinates for anti isomer 7a. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.938137	2.570935	1.255460
2	6	0	0.000000	2.521800	0.694800
3	1	0	-0.838260	2.532087	1.397114
4	1	0	-0.066714	3.417278	0.067789
5	6	0	-0.059545	1.262560	-0.156740
6	1	0	0.784728	1.244832	-0.857231
7	6	0	0.000000	0.000000	0.684788
8	1	0	-0.889054	-0.029959	1.325715
9	1	0	0.889054	0.029959	1.325715
10	6	0	0.059545	-1.262560	-0.156740
11	1	0	-0.784728	-1.244832	-0.857231
12	6	0	0.000000	-2.521800	0.694800
13	1	0	-0.938137	-2.570935	1.255460
14	1	0	0.838260	-2.532087	1.397114
15	1	0	0.066714	-3.417278	0.067789
16	8	0	-1.292118	1.197238	-0.877070
17	1	0	-1.311168	1.963394	-1.455011
18	8	0	1.292118	-1.197238	-0.877070
19	1	0	1.311168	-1.963394	-1.455011

Table 3.12. Optimized Cartesian coordinates for anti isomer 7a. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.968024	2.574924	1.190184
2	6	0	0.000000	2.521938	0.682492
3	1	0	-0.796260	2.524304	1.432924
4	1	0	-0.110379	3.415555	0.059885
5	6	0	-0.098817	1.263361	-0.167131
6	1	0	0.715579	1.251181	-0.903928
7	6	0	0.000000	0.000000	0.670839
8	1	0	-0.886815	-0.054786	1.314426
9	1	0	0.886815	0.054786	1.314426
10	6	0	0.098817	-1.263361	-0.167131
11	1	0	-0.715579	-1.251181	-0.903928
12	6	0	0.000000	-2.521938	0.682492
13	1	0	-0.968024	-2.574924	1.190184
14	1	0	0.796260	-2.524304	1.432924
15	1	0	0.110379	-3.415555	0.059885
16	8	0	-1.360177	1.202235	-0.836656
17	1	0	-1.360950	1.905839	-1.504930
18	8	0	1.360177	-1.202235	-0.836656
19	1	0	1.360950	-1.905839	-1.504930

Table 3.13. Optimized Cartesian coordinates for anti isomer 8. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.325715	-1.496259	1.163777
2	6	0	2.473188	-0.539948	0.653591
3	1	0	2.658587	0.226467	1.415626
4	1	0	3.356178	-0.611370	0.014525
5	6	0	1.255859	-0.167451	-0.179189
6	1	0	1.061422	-0.942312	-0.924665
7	6	0	-0.000001	-0.000112	0.669531
8	1	0	0.128476	0.874251	1.323620
9	1	0	-0.128478	-0.874697	1.323321
10	6	0	-1.255863	0.167521	-0.179130
11	1	0	-1.061437	0.942659	-0.924321
12	6	0	-2.473199	0.539693	0.653786
13	1	0	-2.325732	1.495809	1.164340
14	1	0	-2.658599	-0.227015	1.415526
15	1	0	-3.356186	0.611356	0.014743
16	8	0	1.502895	1.011781	-0.942774
17	1	0	1.725237	1.696245	-0.304997
18	8	0	-1.502882	-1.011432	-0.943152
19	1	0	-1.725191	-1.696142	-0.305627

Table 3.14. Optimized Cartesian coordinates for anti isomer 8. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.314431	1.204843	1.469801
2	6	0	2.470651	0.675131	0.525410
3	1	0	2.651710	1.418221	-0.259821
4	1	0	3.358647	0.044490	0.615526
5	6	0	1.259021	-0.174898	0.170994
6	1	0	1.074863	-0.902009	0.968193
7	6	0	-0.000195	0.665084	-0.009072
8	1	0	0.128475	1.306545	-0.892715
9	1	0	-0.128884	1.328187	0.858449
10	6	0	-1.259395	-0.179192	-0.167812
11	1	0	-1.076618	-0.924054	-0.948782
12	6	0	-2.472217	0.662260	-0.538247
13	1	0	-2.317947	1.171867	-1.493959
14	1	0	-2.652297	1.421831	0.231277
15	1	0	-3.359998	0.029378	-0.613371
16	8	0	1.509448	-0.968863	-0.989232
17	1	0	1.658607	-0.352036	-1.724483
18	8	0	-1.506983	-0.946694	1.010606
19	1	0	-1.657899	-0.313118	1.731245

Table 3.15. Optimized Cartesian coordinates for anti isomer 9a. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.914798	1.978715	-0.223598
2	6	0	-1.662098	1.256980	0.106461
3	1	0	-1.737356	1.290162	1.197746
4	1	0	-2.635254	1.538600	-0.311719
5	6	0	-1.292629	-0.152525	-0.328451
6	1	0	-1.220687	-0.183350	-1.427369
7	6	0	0.024247	-0.659047	0.243193
8	1	0	0.055142	-1.738740	0.058441
9	1	0	0.018974	-0.522985	1.334092
10	6	0	1.283069	-0.027135	-0.341489
11	1	0	1.208350	-0.032602	-1.434275
12	6	0	2.534660	-0.787033	0.077725
13	1	0	2.514371	-1.816791	-0.289617
14	1	0	2.606484	-0.816710	1.170974
15	1	0	3.422377	-0.285276	-0.313611
16	8	0	-2.276324	-1.087407	0.114859
17	1	0	-3.128242	-0.726392	-0.141857
18	8	0	1.404868	1.354947	-0.004704
19	1	0	1.458800	1.387613	0.954917

Table 3.16. Optimized Cartesian coordinates for anti isomer 9a. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.908342	1.977754	-0.229647
2	6	0	-1.662860	1.263525	0.100974
3	1	0	-1.739003	1.305208	1.192107
4	1	0	-2.633328	1.544169	-0.322507
5	6	0	-1.295418	-0.150449	-0.322370
6	1	0	-1.221382	-0.192434	-1.421326
7	6	0	0.022575	-0.648256	0.255817
8	1	0	0.058697	-1.729742	0.079148
9	1	0	0.024118	-0.498014	1.345310
10	6	0	1.282368	-0.025882	-0.339113
11	1	0	1.196365	-0.035049	-1.432975
12	6	0	2.527463	-0.803659	0.068655
13	1	0	2.487393	-1.832266	-0.300980
14	1	0	2.609226	-0.832950	1.161104
15	1	0	3.419373	-0.315920	-0.332184
16	8	0	-2.283818	-1.080624	0.127299
17	1	0	-3.129703	-0.806466	-0.260905
18	8	0	1.423972	1.355320	-0.005362
19	1	0	1.470584	1.406474	0.963574

Table 3.17. Optimized Cartesian coordinates for anti isomer 13. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.897024	1.972828	-0.310878
2	6	0	-1.650291	1.270562	0.046805
3	1	0	-1.697700	1.353504	1.139915
4	1	0	-2.630164	1.532627	-0.359240
5	6	0	-1.306604	-0.158841	-0.342113
6	1	0	-1.258741	-0.237059	-1.433814
7	6	0	0.018125	-0.662057	0.230280
8	1	0	0.056244	-1.739947	0.036695
9	1	0	0.012845	-0.535498	1.324889
10	6	0	1.281801	-0.016570	-0.333496
11	1	0	1.200657	0.019005	-1.425419
12	6	0	2.529043	-0.801676	0.050666
13	1	0	2.499577	-1.816184	-0.356175
14	1	0	2.604813	-0.874103	1.141803
15	1	0	3.419192	-0.291802	-0.324281
16	8	0	-2.361852	-1.045846	0.028341
17	1	0	-2.460238	-0.952054	0.979749
18	8	0	1.415576	1.350023	0.054261
19	1	0	1.488304	1.346758	1.013088

Table 3.18. Optimized Cartesian coordinates for anti isomer 13. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.891317	1.973321	-0.284933
2	6	0	-1.653338	1.273098	0.057937
3	1	0	-1.715164	1.344352	1.150588
4	1	0	-2.625863	1.545013	-0.360562
5	6	0	-1.306067	-0.153187	-0.340879
6	1	0	-1.251572	-0.220863	-1.434877
7	6	0	0.017215	-0.656218	0.233314
8	1	0	0.058019	-1.734075	0.036475
9	1	0	0.012178	-0.529108	1.327534
10	6	0	1.282740	-0.017046	-0.334096
11	1	0	1.201020	0.007728	-1.428262
12	6	0	2.524051	-0.809657	0.056146
13	1	0	2.483723	-1.826499	-0.344630
14	1	0	2.599953	-0.871933	1.147661
15	1	0	3.419005	-0.311907	-0.325124
16	8	0	-2.364519	-1.045387	0.017178
17	1	0	-2.429542	-1.026867	0.985592
18	8	0	1.425272	1.352244	0.043152
19	1	0	1.465931	1.374041	1.013363

Table 3.19. Optimized Cartesian coordinates for anti isomer 15. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.525846	-0.504086	0.086191
2	1	0	-3.213929	-0.152056	-0.686014
3	1	0	-2.792998	-0.021818	1.030603
4	1	0	-2.634634	-1.587586	0.191199
5	6	0	-1.103722	-0.130911	-0.293955
6	1	0	-0.841091	-0.672499	-1.216078
7	6	0	-0.114706	-0.518949	0.803509
8	1	0	-0.366570	0.048839	1.706944
9	1	0	-0.232338	-1.584718	1.033448
10	6	0	1.354535	-0.266904	0.477687
11	6	0	1.830556	-0.957691	-0.791988
12	1	0	1.638251	-2.033400	-0.746653
13	1	0	1.322993	-0.543621	-1.665909
14	1	0	2.908462	-0.813913	-0.923517
15	8	0	-1.092816	1.268130	-0.535839
16	1	0	-0.180993	1.551067	-0.402905
17	8	0	1.515939	1.155675	0.363370
18	1	0	2.407951	1.315057	0.044161
19	1	0	1.955014	-0.624545	1.325804

Table 3.20. Optimized Cartesian coordinates for anti isomer 15. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.535210	-0.463555	0.102812
2	1	0	-3.222396	-0.119829	-0.674965
3	1	0	-2.783824	0.049483	1.036516
4	1	0	-2.669147	-1.540482	0.239507
5	6	0	-1.105522	-0.142228	-0.294800
6	1	0	-0.867068	-0.706166	-1.209263
7	6	0	-0.118986	-0.536042	0.801268
8	1	0	-0.371706	0.022882	1.710944
9	1	0	-0.238220	-1.604191	1.019528
10	6	0	1.350142	-0.277192	0.475756
11	6	0	1.814039	-0.947758	-0.809303
12	1	0	1.617253	-2.023481	-0.777708
13	1	0	1.300865	-0.517801	-1.672788
14	1	0	2.890259	-0.801016	-0.945796
15	8	0	-1.046360	1.256680	-0.569677
16	1	0	-0.124044	1.507588	-0.424477
17	8	0	1.503734	1.148573	0.390610
18	1	0	2.428088	1.343349	0.161742
19	1	0	1.954168	-0.651719	1.314894

Table 3.21. Optimized Cartesian coordinates for anti isomer 15a. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.577857	-1.122668	0.856673
2	6	0	-2.154143	-0.637058	-0.027238
3	1	0	-1.629545	-1.384286	-0.622766
4	1	0	-2.984406	-0.224013	-0.611251
5	6	0	-1.195975	0.470418	0.394420
6	1	0	-1.737378	1.167428	1.048510
7	6	0	0.021534	-0.051550	1.164451
8	1	0	-0.328462	-0.871407	1.800772
9	1	0	0.392361	0.734316	1.831222
10	6	0	1.201499	-0.534657	0.290791
11	1	0	1.717325	-1.331266	0.835628
12	6	0	2.203165	0.582274	0.013568
13	1	0	2.641096	0.950260	0.946666
14	1	0	1.709541	1.415002	-0.491606
15	1	0	3.004793	0.201274	-0.624098
16	8	0	-0.713666	1.193097	-0.750052
17	1	0	-1.489149	1.523641	-1.211217
18	8	0	0.772928	-1.144407	-0.921244
19	1	0	0.351105	-0.424359	-1.404104

Table 3.22. Optimized Cartesian coordinates for anti isomer 15a. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.584611	-1.121750	0.855830
2	6	0	-2.162505	-0.633492	-0.027735
3	1	0	-1.645516	-1.380533	-0.630812
4	1	0	-2.989000	-0.209947	-0.608385
5	6	0	-1.195789	0.466355	0.396983
6	1	0	-1.731818	1.160420	1.059797
7	6	0	0.018928	-0.075253	1.160518
8	1	0	-0.332097	-0.906166	1.782367
9	1	0	0.392078	0.696742	1.842671
10	6	0	1.201236	-0.541213	0.282954
11	1	0	1.715311	-1.352270	0.810924
12	6	0	2.205763	0.579808	0.034011
13	1	0	2.633856	0.929717	0.978541
14	1	0	1.714449	1.420491	-0.459758
15	1	0	3.015380	0.213033	-0.602921
16	8	0	-0.707064	1.193263	-0.740313
17	1	0	-1.474731	1.598631	-1.177958
18	8	0	0.777153	-1.121465	-0.950582
19	1	0	0.320194	-0.399980	-1.403521

Table 3.23. Optimized Cartesian coordinates for anti isomer 23. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.536840	-0.374565	-0.170886
2	1	0	3.239250	-0.049526	0.604188
3	1	0	2.715370	0.218375	-1.071578
4	1	0	2.739053	-1.426769	-0.390481
5	6	0	1.099394	-0.186236	0.286821
6	1	0	0.935992	-0.764419	1.206850
7	6	0	0.098272	-0.636917	-0.765891
8	1	0	0.340843	-0.149214	-1.717006
9	1	0	0.219712	-1.718463	-0.901905
10	6	0	-1.367062	-0.321670	-0.440442
11	6	0	-1.774373	-0.761763	0.962497
12	1	0	-1.563791	-1.823985	1.127608
13	1	0	-1.238713	-0.174165	1.712743
14	1	0	-2.844103	-0.589048	1.100157
15	8	0	0.833985	1.198781	0.547791
16	1	0	1.463659	1.492788	1.210812
17	8	0	-1.658887	1.052075	-0.647226
18	1	0	-0.979419	1.520778	-0.150390
19	1	0	-1.987065	-0.856295	-1.168118

Table 3.24. Optimized Cartesian coordinates for anti isomer 23. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.533529	-0.400002	-0.151860
2	1	0	3.231960	-0.049879	0.614630
3	1	0	2.724863	0.152513	-1.075983
4	1	0	2.720444	-1.463724	-0.327773
5	6	0	1.095639	-0.174014	0.290177
6	1	0	0.918541	-0.721257	1.226028
7	6	0	0.098856	-0.642409	-0.760625
8	1	0	0.349075	-0.169294	-1.718384
9	1	0	0.216564	-1.726035	-0.883182
10	6	0	-1.365522	-0.320278	-0.446463
11	6	0	-1.791971	-0.776229	0.944613
12	1	0	-1.589113	-1.842053	1.093100
13	1	0	-1.258078	-0.206475	1.709941
14	1	0	-2.862614	-0.600276	1.076161
15	8	0	0.848214	1.223159	0.505353
16	1	0	1.320194	1.490697	1.312522
17	8	0	-1.633579	1.069593	-0.625298
18	1	0	-0.925283	1.504553	-0.131873
19	1	0	-1.986816	-0.833193	-1.190679

Table 3.25. Optimized Cartesian coordinates for anti isomer 31. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.526080	-0.464448	-0.123103
2	1	0	3.211767	-0.157333	0.669912
3	1	0	2.773357	0.092722	-1.033894
4	1	0	2.671872	-1.528712	-0.327459
5	6	0	1.089852	-0.180994	0.287937
6	1	0	0.866038	-0.736143	1.202592
7	6	0	0.092599	-0.562712	-0.801516
8	1	0	0.348535	-0.019813	-1.721019
9	1	0	0.203145	-1.633955	-1.012846
10	6	0	-1.373834	-0.259062	-0.472442
11	6	0	-1.830531	-0.887517	0.839943
12	1	0	-1.638807	-1.965518	0.855453
13	1	0	-1.311888	-0.428603	1.686622
14	1	0	-2.901231	-0.717044	0.971697
15	8	0	0.941172	1.195767	0.669220
16	1	0	1.244396	1.710906	-0.085634
17	8	0	-1.628239	1.139375	-0.478573
18	1	0	-1.010093	1.492837	0.170864
19	1	0	-1.985559	-0.662077	-1.286369

Table 3.26. Optimized Cartesian coordinates for anti isomer 31. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.522010	-0.481599	-0.117991
2	1	0	3.209465	-0.181183	0.676648
3	1	0	2.780638	0.067821	-1.030135
4	1	0	2.649544	-1.550180	-0.312828
5	6	0	1.088487	-0.175414	0.286738
6	1	0	0.858164	-0.725859	1.204091
7	6	0	0.091560	-0.554603	-0.804034
8	1	0	0.350152	-0.008112	-1.721155
9	1	0	0.200411	-1.625631	-1.017879
10	6	0	-1.374215	-0.257255	-0.473093
11	6	0	-1.833342	-0.900428	0.830684
12	1	0	-1.638462	-1.977806	0.830391
13	1	0	-1.315663	-0.453043	1.684108
14	1	0	-2.905612	-0.736362	0.963233
15	8	0	0.947788	1.204854	0.660549
16	1	0	1.243604	1.737792	-0.098727
17	8	0	-1.628141	1.147582	-0.457271
18	1	0	-0.969198	1.498122	0.155721
19	1	0	-1.987218	-0.649244	-1.293508

Table 3.27. Optimized Cartesian coordinates for anti isomer 91. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.464023	-1.623294	-0.904844
2	6	0	2.509669	-0.771170	-0.220528
3	1	0	2.668401	-1.158209	0.792417
4	1	0	3.362609	-0.144022	-0.489448
5	6	0	1.223313	0.034595	-0.278313
6	1	0	1.094257	0.446336	-1.281773
7	6	0	-0.009935	-0.801115	0.053886
8	1	0	0.177777	-1.399917	0.956649
9	1	0	-0.188858	-1.501311	-0.771572
10	6	0	-1.255995	0.064095	0.277866
11	1	0	-1.196670	0.493866	1.287328
12	6	0	-2.531848	-0.746370	0.160247
13	1	0	-2.510470	-1.602224	0.841061
14	1	0	-2.632818	-1.113755	-0.864885
15	1	0	-3.400222	-0.126261	0.393278
16	8	0	1.304485	1.193331	0.560569
17	1	0	1.428768	0.870671	1.458076
18	8	0	-1.334381	1.112735	-0.678980
19	1	0	-0.638854	1.729388	-0.427949

Table 3.28. Optimized Cartesian coordinates for anti isomer 91. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.416692	-1.524036	-1.093746
2	6	0	2.500993	-0.764071	-0.311027
3	1	0	2.659092	-1.271951	0.646935
4	1	0	3.371807	-0.137027	-0.518563
5	6	0	1.241929	0.087400	-0.248595
6	1	0	1.109714	0.605243	-1.204327
7	6	0	-0.002734	-0.750043	0.019632
8	1	0	0.165960	-1.375597	0.908346
9	1	0	-0.168104	-1.422569	-0.832222
10	6	0	-1.255274	0.093986	0.245199
11	1	0	-1.156114	0.616664	1.205435
12	6	0	-2.506584	-0.764141	0.267314
13	1	0	-2.415964	-1.558759	1.013324
14	1	0	-2.651060	-1.222529	-0.715780
15	1	0	-3.384538	-0.156674	0.500320
16	8	0	1.375407	1.138073	0.709767
17	1	0	1.438897	0.719632	1.584654
18	8	0	-1.425080	1.049837	-0.802097
19	1	0	-0.858970	1.805536	-0.590867

Table 3.29. Optimized Cartesian coordinates for anti isomer 92. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.512256	-1.598213	-0.839536
2	6	0	2.534258	-0.737920	-0.164390
3	1	0	2.645712	-1.097778	0.862564
4	1	0	3.397441	-0.114884	-0.408709
5	6	0	1.253456	0.064967	-0.279119
6	1	0	1.176519	0.489576	-1.287487
7	6	0	0.014644	-0.805099	-0.040631
8	1	0	0.197262	-1.485399	0.800095
9	1	0	-0.172651	-1.414132	-0.933938
10	6	0	-1.220073	0.023715	0.279138
11	1	0	-1.104637	0.424733	1.294485
12	6	0	-2.502876	-0.784798	0.194202
13	1	0	-2.463147	-1.643122	0.870969
14	1	0	-2.643113	-1.144567	-0.828634
15	1	0	-3.370849	-0.176431	0.470906
16	8	0	1.332727	1.120770	0.673662
17	1	0	0.642031	1.735793	0.407989
18	8	0	-1.237748	1.112233	-0.654523
19	1	0	-2.053117	1.595217	-0.497016

Table 3.30. Optimized Cartesian coordinates for anti isomer 92. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.512256	-1.598213	-0.839536
2	6	0	2.534258	-0.737920	-0.164390
3	1	0	2.645712	-1.097778	0.862564
4	1	0	3.397441	-0.114884	-0.408709
5	6	0	1.253456	0.064967	-0.279119
6	1	0	1.176519	0.489576	-1.287487
7	6	0	0.014644	-0.805099	-0.040631
8	1	0	0.197262	-1.485399	0.800095
9	1	0	-0.172651	-1.414132	-0.933938
10	6	0	-1.220073	0.023715	0.279138
11	1	0	-1.104637	0.424733	1.294485
12	6	0	-2.502876	-0.784798	0.194202
13	1	0	-2.463147	-1.643122	0.870969
14	1	0	-2.643113	-1.144567	-0.828634
15	1	0	-3.370849	-0.176431	0.470906
16	8	0	1.332727	1.120770	0.673662
17	1	0	0.642031	1.735793	0.407989
18	8	0	-1.237748	1.112233	-0.654523
19	1	0	-2.053117	1.595217	-0.497016

Table 3.31. Optimized Cartesian coordinates for syn isomer 1. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.508256	-1.882138	0.115099
2	6	0	-2.512823	-0.827042	-0.172973
3	1	0	-2.540942	-0.754546	-1.263194
4	1	0	-3.423357	-0.369362	0.227828
5	6	0	-1.274520	-0.118314	0.351884
6	1	0	-1.247341	-0.188978	1.449792
7	6	0	0.014556	-0.710142	-0.195120
8	1	0	0.005806	-0.639441	-1.289898
9	1	0	0.039945	-1.771714	0.078081
10	6	0	1.278926	-0.021073	0.319604
11	1	0	1.193384	0.071777	1.416016
12	6	0	2.527480	-0.818737	-0.009640
13	1	0	2.587134	-0.976993	-1.090154
14	1	0	2.519227	-1.788930	0.495059
15	1	0	3.412465	-0.261295	0.305643
16	8	0	-1.292402	1.264563	-0.030668
17	1	0	-2.054987	1.669038	0.390316
18	8	0	1.447187	1.259534	-0.266072
19	1	0	0.576929	1.671654	-0.223204

Table 3.32. Optimized Cartesian coordinates for syn isomer 1. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.500430	-1.881100	0.194684
2	6	0	-2.506629	-0.842093	-0.148158
3	1	0	-2.530890	-0.828126	-1.241445
4	1	0	-3.415433	-0.360684	0.225841
5	6	0	-1.270667	-0.106236	0.344693
6	1	0	-1.238893	-0.132338	1.444659
7	6	0	0.017107	-0.718376	-0.186314
8	1	0	0.013916	-0.662446	-1.283167
9	1	0	0.035458	-1.776859	0.099653
10	6	0	1.281348	-0.034626	0.329420
11	1	0	1.209832	0.030362	1.428782
12	6	0	2.534019	-0.807892	-0.038564
13	1	0	2.583352	-0.934837	-1.124189
14	1	0	2.537742	-1.793123	0.435912
15	1	0	3.420519	-0.256644	0.286143
16	8	0	-1.295532	1.262086	-0.093681
17	1	0	-1.952140	1.735085	0.446440
18	8	0	1.418569	1.272991	-0.221340
19	1	0	0.521606	1.635433	-0.199617

Table 3.33. Optimized Cartesian coordinates for syn isomer 3. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.832275	-1.206613	-0.625954
2	6	0	2.543216	-0.402846	0.056936
3	1	0	2.560690	-0.782480	1.081964
4	1	0	3.286775	0.396972	-0.029941
5	6	0	1.152865	0.111097	-0.275226
6	1	0	1.145327	0.531116	-1.288856
7	6	0	0.102780	-0.987490	-0.215435
8	1	0	0.218520	-1.545052	0.721689
9	1	0	0.316443	-1.679243	-1.037914
10	6	0	-1.345151	-0.460385	-0.331207
11	1	0	-1.936540	-1.194677	-0.886308
12	6	0	-1.991671	-0.250449	1.033304
13	1	0	-1.402284	0.455461	1.622611
14	1	0	-2.051222	-1.195558	1.582058
15	1	0	-3.002171	0.145449	0.903875
16	8	0	0.755940	1.132322	0.652684
17	1	0	1.461582	1.784701	0.661031
18	8	0	-1.412084	0.723357	-1.118349
19	1	0	-0.952472	1.384930	-0.589165

Table 3.34. Optimized Cartesian coordinates for syn isomer 3. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.826729	-1.210679	-0.627313
2	6	0	2.545039	-0.405579	0.057864
3	1	0	2.561932	-0.787345	1.082565
4	1	0	3.289035	0.393072	-0.027771
5	6	0	1.155642	0.116491	-0.270321
6	1	0	1.152338	0.531553	-1.287599
7	6	0	0.107622	-0.985571	-0.208463
8	1	0	0.224464	-1.543584	0.728890
9	1	0	0.322413	-1.679553	-1.029349
10	6	0	-1.342763	-0.472067	-0.319887
11	1	0	-1.935632	-1.223633	-0.853121
12	6	0	-1.980668	-0.235695	1.043989
13	1	0	-1.393409	0.490108	1.610210
14	1	0	-2.024086	-1.169321	1.613361
15	1	0	-2.997930	0.144902	0.916423
16	8	0	0.758717	1.139666	0.651395
17	1	0	1.388637	1.873689	0.554068
18	8	0	-1.429129	0.697387	-1.134481
19	1	0	-0.960433	1.378885	-0.634768

Table 3.33. Optimized Cartesian coordinates for syn isomer 23. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.542775	-1.823799	0.301299
2	6	0	-2.534330	-0.807075	-0.101246
3	1	0	-2.567414	-0.854266	-1.193410
4	1	0	-3.424766	-0.279173	0.247563
5	6	0	-1.290999	-0.057048	0.338995
6	1	0	-1.244325	-0.060448	1.441212
7	6	0	-0.014440	-0.714018	-0.185066
8	1	0	-0.018246	-0.651055	-1.282399
9	1	0	-0.020022	-1.777070	0.086402
10	6	0	1.270095	-0.086802	0.348235
11	1	0	1.227532	-0.070405	1.442438
12	6	0	2.515060	-0.835016	-0.100209
13	1	0	2.560822	-0.864657	-1.194806
14	1	0	2.506437	-1.865001	0.266458
15	1	0	3.410471	-0.332068	0.271990
16	8	0	-1.425161	1.272872	-0.138262
17	1	0	-0.565134	1.682225	0.012921
18	8	0	1.363840	1.299776	-0.016018
19	1	0	1.495673	1.314287	-0.969678

Table 3.34. Optimized Cartesian coordinates for syn isomer 23. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.545180	-1.822542	-0.293931
2	6	0	2.535517	-0.804627	0.105393
3	1	0	2.568562	-0.850594	1.198027
4	1	0	3.427149	-0.279297	-0.246849
5	6	0	1.289007	-0.062951	-0.339475
6	1	0	1.239597	-0.074135	-1.441666
7	6	0	0.015432	-0.714276	0.194013
8	1	0	0.017468	-0.646324	1.291377
9	1	0	0.020990	-1.777888	-0.075806
10	6	0	-1.266586	-0.086226	-0.344507
11	1	0	-1.215268	-0.069649	-1.440284
12	6	0	-2.512161	-0.839964	0.091985
13	1	0	-2.566907	-0.873122	1.185873
14	1	0	-2.494396	-1.867157	-0.282653
15	1	0	-3.406791	-0.339404	-0.286530
16	8	0	1.415654	1.280976	0.120898
17	1	0	0.531375	1.658439	0.018310
18	8	0	-1.358437	1.300933	0.022053
19	1	0	-1.491948	1.334667	0.986062

Table 3.35. Optimized Cartesian coordinates for syn isomer 34. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.846794	-1.063897	-0.762863
2	6	0	2.546265	-0.369288	0.026668
3	1	0	2.531987	-0.903095	0.981262
4	1	0	3.281446	0.435895	0.091251
5	6	0	1.168931	0.200533	-0.252767
6	1	0	1.201562	0.792798	-1.176018
7	6	0	0.134538	-0.914321	-0.452135
8	1	0	0.279655	-1.687528	0.311279
9	1	0	0.328372	-1.375837	-1.427178
10	6	0	-1.319628	-0.433816	-0.386327
11	1	0	-1.930352	-1.075055	-1.036094
12	6	0	-1.894916	-0.484926	1.023438
13	1	0	-1.267609	0.088473	1.706676
14	1	0	-1.938949	-1.520222	1.374047
15	1	0	-2.913635	-0.081443	1.040343
16	8	0	0.839880	1.053053	0.838729
17	1	0	0.065575	1.534344	0.528495
18	8	0	-1.344361	0.905977	-0.903017
19	1	0	-2.260134	1.194242	-0.870164

Table 3.36. Optimized Cartesian coordinates for syn isomer 34. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.838758	-1.054650	-0.790667
2	6	0	2.545915	-0.375554	0.014962
3	1	0	2.534428	-0.931999	0.957098
4	1	0	3.287436	0.423767	0.090847
5	6	0	1.169017	0.203547	-0.248379
6	1	0	1.202386	0.814307	-1.160562
7	6	0	0.132099	-0.904116	-0.464528
8	1	0	0.276227	-1.692733	0.283908
9	1	0	0.329063	-1.346999	-1.448176
10	6	0	-1.322349	-0.422335	-0.394143
11	1	0	-1.932652	-1.048810	-1.059734
12	6	0	-1.898812	-0.510410	1.014129
13	1	0	-1.273457	0.046368	1.713277
14	1	0	-1.941632	-1.555095	1.337020
15	1	0	-2.915701	-0.104417	1.037851
16	8	0	0.847029	1.043665	0.860154
17	1	0	0.056329	1.519070	0.574455
18	8	0	-1.340307	0.928628	-0.877570
19	1	0	-2.270177	1.206052	-0.928241

Table 3.37. Optimized Cartesian coordinates for syn isomer 45. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.892529	1.919150	0.705858
2	6	0	-1.626000	1.110385	0.732399
3	1	0	-1.667216	0.690328	1.742200
4	1	0	-2.608354	1.521457	0.488922
5	6	0	-1.271567	0.030806	-0.270797
6	1	0	-1.144562	0.489755	-1.258407
7	6	0	0.009083	-0.719396	0.088061
8	1	0	0.210838	-1.469596	-0.689303
9	1	0	-0.164467	-1.255506	1.028623
10	6	0	1.238668	0.161043	0.227977
11	1	0	1.097376	0.830618	1.088877
12	6	0	2.503951	-0.655912	0.442737
13	1	0	2.671470	-1.305973	-0.420263
14	1	0	2.422633	-1.271033	1.343563
15	1	0	3.374874	-0.001488	0.557071
16	8	0	-2.374139	-0.877009	-0.287474
17	1	0	-2.149456	-1.562971	-0.920756
18	8	0	1.323643	0.927755	-0.972315
19	1	0	2.128558	1.447733	-0.910332

Table 3.38. Optimized Cartesian coordinates for syn isomer 45. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.896581	1.907535	0.749489
2	6	0	-1.635877	1.103547	0.750258
3	1	0	-1.689500	0.668539	1.753535
4	1	0	-2.612089	1.528243	0.502490
5	6	0	-1.273998	0.035955	-0.264111
6	1	0	-1.147424	0.506660	-1.247381
7	6	0	0.009305	-0.709783	0.091963
8	1	0	0.199719	-1.469594	-0.679181
9	1	0	-0.153940	-1.236840	1.040174
10	6	0	1.243553	0.168817	0.214588
11	1	0	1.103134	0.866439	1.053280
12	6	0	2.496929	-0.656299	0.471033
13	1	0	2.660218	-1.344917	-0.362934
14	1	0	2.399726	-1.232446	1.396227
15	1	0	3.373876	-0.007056	0.561392
16	8	0	-2.373673	-0.876733	-0.299028
17	1	0	-2.171465	-1.529532	-0.988874
18	8	0	1.349770	0.897662	-1.007681
19	1	0	2.086080	1.522121	-0.906934

Table 3.39. Optimized Cartesian coordinates for syn isomer 71. MP2/6-311G(d,p) gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.443697	-1.343258	1.248644
2	6	0	-2.510410	-0.671335	0.388126
3	1	0	-2.673290	-1.264075	-0.515880
4	1	0	-3.376862	-0.017349	0.535113
5	6	0	-1.235536	0.144865	0.237832
6	1	0	-1.101019	0.761524	1.138814
7	6	0	-0.015505	-0.741400	0.060171
8	1	0	-0.207909	-1.462065	-0.742438
9	1	0	0.156031	-1.308234	0.983028
10	6	0	1.259997	0.016662	-0.274334
11	1	0	1.136043	0.484519	-1.258394
12	6	0	1.601340	1.091824	0.746763
13	1	0	1.665274	0.653925	1.747519
14	1	0	0.853936	1.889007	0.742313
15	1	0	2.570870	1.542804	0.509400
16	8	0	-1.301741	0.985404	-0.913913
17	1	0	-2.111377	1.495596	-0.834704
18	8	0	2.282495	-0.979002	-0.325258
19	1	0	3.086656	-0.527301	-0.591393

Table 3.40. Optimized Cartesian coordinates for syn isomer 71. MP2/6-311G(d,p) PCM (CH₂Cl₂).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.414061	-1.329211	1.289156
2	6	0	-2.501330	-0.682885	0.410491
3	1	0	-2.664095	-1.304213	-0.474781
4	1	0	-3.374047	-0.035755	0.545489
5	6	0	-1.239863	0.148962	0.224782
6	1	0	-1.101532	0.782461	1.113143
7	6	0	-0.014571	-0.731857	0.048437
8	1	0	-0.203831	-1.447986	-0.760660
9	1	0	0.145632	-1.306741	0.969332
10	6	0	1.267149	0.023995	-0.268399
11	1	0	1.156579	0.503499	-1.249393
12	6	0	1.601069	1.086579	0.768631
13	1	0	1.642940	0.638259	1.766361
14	1	0	0.857449	1.887683	0.763582
15	1	0	2.577875	1.529760	0.549291
16	8	0	-1.331611	0.967123	-0.941086
17	1	0	-2.061339	1.590675	-0.797186
18	8	0	2.291958	-0.971499	-0.324695
19	1	0	3.080935	-0.542191	-0.691740