Supporting information for

How many solvent molecules are required to solvate chiral 1,2-diols with hydrogen bonding solvents? A VCD spectroscopic study

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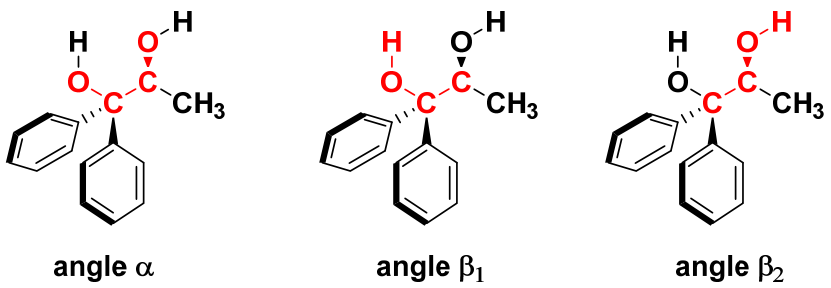
Table S1. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated (S)-1** calculated within the **IEFPCM of chloroform**.

Conf.-id	ΔE_{ZPC}[a] [kcal/mol]	ΔG_{298K}[a] [kcal/mol]	pop-ΔE_{ZPC} [%]	pop-ΔG [%]	α [deg]	β_1 [deg]	β_2 [deg]
1-c6	0.00	0.00	64.4	53.1	-57.1	44.8	-66.7
1-c1	0.73	0.36	18.9	29.1	-58.5	49.5	160.5
1-c5	1.34	1.22	6.7	6.7	-56.1	144.3	47.8
1-c2	1.99	1.82	2.2	2.4	-59.6	-75.4	48.4
1-c11	2.28	2.21	1.4	1.3	-177.3	-75.9	71.3
1-c13	2.31	2.15	1.3	1.4	177.8	-157.4	74.7
1-c12	2.38	2.00	1.2	1.8	-61.9	-64.3	-52.7
1-c10	2.64	2.51	0.7	0.8	169.5	72.4	-58.5
1-c17	2.71	2.40	0.7	0.9	168.8	-159.4	-64.1
1-c23	2.72	2.88	0.6	0.4	47.3	82.8	-42.6
1-c24	2.76	3.08	0.6	0.3	48.4	-34.2	77.1
1-c19	2.79	2.72	0.6	0.5	53.9	173.5	-49.7
1-c16	3.19	2.78	0.3	0.5	174.7	-157.8	162.5
1-c18	3.91	4.03	0.1	0.1	49.8	-36.2	-156.7
1-c8	3.99	3.87	0.1	0.1	-63.8	-168.7	-52.1
1-c14	4.15	4.04	0.1	0.1	171.9	-46.1	-59.1
1-c9	4.23	3.69	0.1	0.1	170.4	74.5	-168.5
1-c7	4.53	3.61	0.0	0.1	-63.2	-55.6	179.3
1-c4	4.56	4.40	0.0	0.0	50.5	62.4	63.9
1-c21	4.57	4.62	0.0	0.0	57.7	165.0	65.6
1-c15	5.73	5.56	0.0	0.0	172.8	-53.4	179.6
1-c20	6.05	5.80	0.0	0.0	60.4	166.2	-168.1
1-c22	6.11	5.64	0.0	0.0	49.4	61.9	166.3

[a] referenced to E_{ZPC}= -731.624238 hartree and G= -731.666541 hartree



Scheme S1. Angle definition for diphenyl-propylene-1,2-diol (S)-**1**

Table S2. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated (S)-1** calculated within the **IEFPCM of acetonitrile**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
1-c6	0.0	0.0	57.3	47.7	-57.0	45.7	-68.2
1-c1	0.5	0.2	24.7	35.5	-58.5	47.6	161.9
1-c5	1.4	1.4	5.3	4.6	-56.4	146.3	47.4
1-c2	1.5	1.6	4.2	3.5	-59.1	-75.4	50.0
1-c12	2.0	1.5	1.8	3.6	-62.5	-68.1	-57.4
1-c11	2.4	2.5	1.0	0.7	-177.7	-71.8	72.8
1-c13	2.5	2.5	0.9	0.7	177.2	-163.1	75.6
1-c23	2.5	2.7	0.9	0.5	47.7	80.4	-43.4
1-c24	2.5	2.9	0.8	0.3	48.1	-35.1	78.0
1-c19	2.6	2.8	0.7	0.4	54.3	177.9	-48.8
1-c10	2.7	2.7	0.6	0.5	168.9	71.9	-59.0
1-c17	2.7	2.5	0.6	0.7	169.0	-159.7	-64.1
1-c16	3.1	2.8	0.3	0.4	175.5	-163.0	173.1
1-c18	3.3	3.6	0.2	0.1	50.4	-36.2	-153.9
1-c8	3.4	3.4	0.2	0.2	-63.9	-169.9	-56.1
1-c7	3.4	3.0	0.2	0.3	-62.6	-58.3	-177.5
1-c3	3.7	3.3	0.1	0.2	-62.7	160.7	178.8
1-c9	3.9	3.8	0.1	0.1	168.4	72.3	-175.2
1-c14	4.0	4.0	0.1	0.1	172.2	-46.1	-61.0
1-c21	4.1	4.3	0.1	0.0	57.5	168.4	67.2
1-c4	4.3	4.4	0.0	0.0	52.0	65.4	66.6
1-c15	5.2	4.9	0.0	0.0	172.4	-49.9	180.0
1-c20	5.3	5.3	0.0	0.0	60.5	168.1	-171.8
1-c22	5.5	5.2	0.0	0.0	53.6	64.9	178.1

[a] referenced to E_{ZPC}= -731.626963 hartree and G= -731.669500 hartree

Table S3. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated (S)-1** calculated within the **IEFPCM of DMSO**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
1-c6	0.0	0.0	56.9	46.7	-57.0	45.8	-68.3
1-c1	0.5	0.2	25.0	35.7	-58.6	47.5	162.0
1-c5	1.4	1.4	5.3	4.5	-56.4	146.4	47.4
1-c2	1.5	1.5	4.3	3.5	-59.0	-75.3	50.1
1-c12	2.0	1.4	1.9	4.4	-62.5	-68.3	-57.8
1-c11	2.4	2.5	1.0	0.7	-177.8	-71.6	72.9
1-c23	2.5	2.7	0.9	0.5	47.8	80.3	-43.5
1-c13	2.5	2.5	0.9	0.7	177.2	-163.3	75.7
1-c24	2.5	2.9	0.8	0.3	48.1	-35.1	78.1
1-c19	2.6	2.8	0.7	0.4	54.3	178.1	-48.7
1-c10	2.7	2.7	0.6	0.5	168.9	71.9	-59.0
1-c17	2.7	2.5	0.5	0.7	169.0	-159.8	-64.1
1-c16	3.1	2.8	0.3	0.4	175.5	-163.3	173.5
1-c18	3.3	3.6	0.2	0.1	50.5	-36.2	-153.8
1-c8	3.3	3.3	0.2	0.2	-63.9	-169.9	-56.3
1-c7	3.4	3.0	0.2	0.3	-62.6	-58.4	-177.4
1-c3	3.7	3.3	0.1	0.2	-62.6	161.9	179.3
1-c9	3.9	3.8	0.1	0.1	168.4	72.3	-175.4
1-c14	4.0	4.1	0.1	0.0	172.3	-46.1	-61.1
1-c21	4.1	4.3	0.1	0.0	57.5	168.6	67.3
1-c4	4.3	4.4	0.0	0.0	52.0	65.5	66.7
1-c15	5.2	4.9	0.0	0.0	172.4	-49.7	180.0
1-c20	5.3	5.2	0.0	0.0	60.5	168.2	-171.8
1-c22	5.4	5.2	0.0	0.0	53.8	65.0	178.5

[a] referenced to E_{ZPC}= -731.627083 hartree and G= -731.669623 hartree

Table S4. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **ACN-monosolvated (S)-1** calculated within the **IEFPCM of acetonitrile**. The H-bond donaring OH-group is denoted with @S/@T.

Conf.	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
1-c1··ACN$^{@S}$	0.0	0.0	41.1	49.5	-57.1	44.9	172.4
1-c6··ACN$^{@S}$	0.3	0.7	25.8	15.6	-51.5	44.4	-94.9
1-c6··ACN$^{@T}$	0.8	1.0	10.8	9.2	-62.3	60.5	-61.9
1-c2··ACN$^{@T}$	1.3	2.1	4.9	1.3	-57.4	-76.7	47.4
1-c1··ACN$^{@T}$	1.5	1.2	3.4	6.7	-63.5	62.6	166.4
1-c5··ACN$^{@T}$	1.6	1.3	2.7	5.7	-54.6	164.6	43.3
1-c23··ACN$^{@T}$	2.0	2.8	1.4	0.5	46.2	76.0	-39.9
1-c11··ACN$^{@T}$	2.1	2.4	1.2	0.9	-177.0	-67.1	70.7
1-c12··ACN$^{@T}$	2.1	2.3	1.2	1.1	-61.9	-73.4	-55.9
1-c18··ACN$^{@S}$	2.2	2.1	1.0	1.5	48.2	-34.6	-143.7
1-c2··ACN$^{@S}$	2.3	2.4	0.8	0.8	-63.7	-71.5	68.6
1-c24··ACN$^{@S}$	2.5	3.2	0.6	0.2	44.4	-34.8	91.1
1-c19··ACN$^{@T}$	2.5	3.1	0.6	0.3	53.1	-178.2	-45.3
1-c17··ACN$^{@T}$	2.5	3.1	0.6	0.3	168.3	-162.8	-62.8
1-c15··ACN$^{@S}$	2.7	2.2	0.4	1.2	-179.0	-71.7	-171.5
1-c13··ACN$^{@T}$	2.7	3.3	0.4	0.2	175.5	-172.8	75.3
1-c16··ACN$^{@S}$	2.8	1.9	0.4	2.0	176.9	-164.8	-168.4
1-c15··ACN$^{@T}$	2.8	2.7	0.3	0.5	-179.3	-68.2	175.9
1-c7··ACN$^{@S}$	2.9	2.7	0.3	0.5	-63.1	-67.0	-163.9
1-c11··ACN$^{@S}$	2.9	3.2	0.3	0.2	179.5	-71.2	95.9
1-c13··ACN$^{@S}$	3.0	3.6	0.2	0.1	174.9	-164.0	97.5
1-c17··ACN$^{@S}$	3.1	3.0	0.2	0.3	172.5	-158.2	-88.5
1-c8··ACN$^{@T}$	3.2	3.6	0.2	0.1	-63.9	-171.1	-54.5
1-c9··ACN$^{@S}$	3.3	2.9	0.1	0.4	170.5	71.6	-154.3
1-c7··ACN$^{@T}$	3.4	3.6	0.1	0.1	-63.8	-73.8	-178.0
1-c16··ACN$^{@T}$	3.4	3.6	0.1	0.1	172.2	-169.6	172.4
1-c23··ACN$^{@S}$	3.5	3.6	0.1	0.1	51.6	74.1	-63.0
1-c19··ACN$^{@S}$	3.6	3.6	0.1	0.1	58.1	173.4	-69.0
1-c14··ACN$^{@T}$	3.6	4.3	0.1	0.0	172.2	-44.4	-59.6
1-c24··ACN$^{@T}$	3.9	4.0	0.1	0.1	52.2	-43.0	75.4
1-c9··ACN$^{@S}$	4.0	4.2	0.0	0.0	167.8	74.3	-176.5
1-c3··ACN$^{@T}$	4.0	4.1	0.0	0.1	-64.5	-172.7	177.4
1-c14··ACN$^{@S}$	4.2	4.3	0.0	0.0	173.6	-49.3	-94.7
1-c4··ACN$^{@T}$	4.2	4.1	0.0	0.1	50.9	59.6	64.6
1-c21··ACN$^{@T}$	4.3	3.7	0.0	0.1	59.5	171.9	65.2
1-c18··ACN$^{@T}$	4.8	4.3	0.0	0.0	54.7	-43.2	-152.0
1-c21··ACN$^{@S}$	5.0	5.5	0.0	0.0	57.1	168.1	87.5
1-c4··ACN$^{@S}$	5.1	5.7	0.0	0.0	51.2	62.7	88.4
1-c22··ACN$^{@T}$	5.4	5.2	0.0	0.0	52.1	58.9	178.1
1-c20··ACN$^{@T}$	5.6	5.9	0.0	0.0	63.7	170.9	-169.3

[a] referenced to E_{ZPC}= -864.402240 hartree and G= -864.457336 hartree

Table S5. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **ACN-twofold solvated (S)-1** calculated within the **IEFPCM of acetonitrile**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
1-c1··$(ACN)_2$	0.0	0.0	60.5	45.8	-62.2	61.1	-178.3
1-c2··$(ACN)_2$	1.2	1.8	8.3	2.2	-63.0	-75.1	64.4
1-c15··$(ACN)_2$	1.4	1.6	5.3	3.3	-177.8	-66.7	-170.5
1-c11··$(ACN)_2$	1.6	2.5	4.0	0.6	-179.9	-67.1	95.1
1-c5··$(ACN)_2$	1.7	1.4	3.3	4.5	-63.0	-179.5	67.7
1-c12··$(ACN)_2$	1.9	2.5	2.5	0.7	-61.0	-73.1	-93.4
1-c17··$(ACN)_2$	1.9	1.9	2.5	1.9	171.7	-162.7	-91.2
1-c7··$(ACN)_2$	1.9	1.9	2.5	1.7	-62.8	-72.4	-161.8
1-c16··$(ACN)_2$	1.9	0.3	2.4	27.6	174.0	-170.1	-166.5
1-c10··$(ACN)_2$	2.2	3.4	1.6	0.1	169.9	74.1	-90.4
1-c13··$(ACN)_2$	2.2	2.5	1.5	0.7	172.7	-171.4	98.8
1-c23··$(ACN)_2$	2.3	2.0	1.2	1.6	50.7	74.6	-55.0
1-c9··$(ACN)_2$	2.4	1.7	1.1	2.5	170.0	75.0	-154.3
1-c19··$(ACN)_2$	2.5	1.9	0.8	1.8	58.5	177.5	-63.7
1-c8··$(ACN)_2$	2.7	2.7	0.6	0.5	-63.6	-173.6	-167.6
1-c14··$(ACN)_2$	2.7	2.7	0.6	0.5	173.5	-45.8	-92.6
1-c18··$(ACN)_2$	2.8	1.6	0.5	3.3	52.5	-41.3	-141.3
1-c24··$(ACN)_2$	3.1	2.6	0.3	0.5	48.5	-42.1	90.7
1-c22··$(ACN)_2$	4.0	3.1	0.1	0.3	54.9	58.4	-151.5
1-c4··$(ACN)_2$	4.0	5.0	0.1	0.0	50.8	58.3	88.3
1-c21··$(ACN)_2$	4.1	4.9	0.1	0.0	59.3	171.4	86.1

[a] referenced to E_{ZPC}= -997.175623 hartree and G= -997.243074 hartree

Table S6. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **DMSO-monosolvated (S)-1** calculated within the **IEFPCM of DMSO**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
1-c5··DMSO_bifu	0.0	0.56	59.2	15.5	-70.4	58.3	57.8
1-c1··DMSO$^{@S}$	0.6	0.00	20.6	40.0	-56.2	43.6	175.0
1-c6··DMSO$^{@S}$	1.1	0.03	10.0	37.9	-51.0	44.4	-102.7
1-c6··DMSO$^{@T}$	1.6	2.2	3.8	0.9	-64.0	62.3	-61.9
1-c2··DMSO$^{@T}$	2.2	2.3	1.3	0.8	-55.9	-75.4	45.3
1-c1··DMSO$^{@T}$	2.4	3.0	1.1	0.3	-64.5	67.2	170.5
1-c5··DMSO$^{@T}$	2.4	2.2	1.1	1.0	-55.3	177.7	43.9
1-c18··DMSO$^{@S}$	2.6	2.2	0.7	1.0	47.0	-33.4	-143.7
1-c23··DMSO$^{@T}$	2.8	3.2	0.5	0.2	45.7	73.8	-38.5
1-c19··DMSO$^{@T}$	3.5	4.0	0.2	0.0	52.2	-178.0	-43.9
1-c17··DMSO$^{@T}$	3.5	3.2	0.2	0.2	168.3	-164.4	-62.2
1-c15··DMSO$^{@T}$	3.6	3.5	0.1	0.1	-178.6	-66.9	177.2
1-c10··DMSO$^{@T}$	3.6	3.5	0.1	0.1	167.5	74.5	-57.4
1-c15··DMSO$^{@S}$	3.6	2.2	0.1	0.9	-179.0	-69.7	-169.2
1-c13··DMSO$^{@T}$	3.6	3.9	0.1	0.1	174.7	-175.1	75.8
1-c7··DMSO$^{@S}$	3.6	3.0	0.1	0.3	-62.3	-56.3	-164.3
1-c23··DMSO_bifu	3.8	4.3	0.1	0.0	46.0	30.0	-77.6
1-c14··DMSO$^{@T}$	3.8	3.6	0.1	0.1	175.1	-63.3	-60.8
1-c8··DMSO$^{@T}$	4.0	4.3	0.1	0.0	-64.6	-171.5	-54.6
1-c16··DMSO$^{@S}$	4.0	3.5	0.1	0.1	171.4	-159.4	-150.2
1-c10··DMSO$^{@S}$	4.2	4.1	0.1	0.0	170.7	70.3	-98.9
1-c17··DMSO$^{@S}$	4.2	3.9	0.1	0.1	172.4	-157.7	-100.2
1-c13··DMSO$^{@S}$	4.2	3.7	0.0	0.1	174.1	-163.8	103.6
1-c9··DMSO$^{@S}$	4.2	3.3	0.0	0.2	170.1	69.7	-157.1
1-c7··DMSO$^{@T}$	4.2	4.3	0.0	0.0	-63.7	-75.1	-178.7
1-c16··DMSO$^{@T}$	4.5	4.2	0.0	0.0	172.5	-170.3	172.9
1-c19··DMSO$^{@S}$	4.5	4.9	0.0	0.0	58.7	173.4	-76.8
1-c9··DMSO$^{@T}$	4.7	4.5	0.0	0.0	167.3	73.3	-177.0
1-c12··DMSO$^{@T}$	4.9	5.0	0.0	0.0	51.1	54.9	64.0
1-c4··DMSO$^{@T}$	5.0	5.3	0.0	0.0	-65.0	-172.2	177.6
1-c14··DMSO$^{@S}$	5.2	5.0	0.0	0.0	173.4	-47.5	-99.4
1-c12··DMSO$^{@T}$	5.3	6.1	0.0	0.0	49.7	52.5	63.8
1-c21··DMSO$^{@T}$	5.3	5.6	0.0	0.0	59.7	173.2	65.0
1-c21··DMSO$^{@S}$	6.1	5.7	0.0	0.0	56.6	168.2	91.3
1-c22··DMSO$^{@T}$	6.1	5.7	0.0	0.0	52.9	55.7	179.9
1-c18··DMSO$^{@T}$	6.4	5.8	0.0	0.0	57.4	-49.8	-149.2
1-c20··DMSO$^{@T}$	6.6	6.2	0.0	0.0	63.6	169.7	-170.9

[a] referenced to E_{ZPC}= -1284.873270 hartree and G= -1284.929795 hartree

Table S7. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **DMSO-twofold solvated (S)-1** calculated within the **IEFPCM of DMSO**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
1-c1··$(DMSO)_2$	0.0	0.0	72.0	49.9	-62.4	66.7	-162.6
1-c15··$(DMSO)_2$	1.5	1.2	6.2	7.0	-176.4	-63.3	-165.9
1-c2··$(DMSO)_2$	1.7	1.6	3.8	3.2	-64.7	-77.2	75.9
1-c16··$(DMSO)_2$	1.9	1.4	2.7	4.4	170.9	-163.2	-150.9
1-c17··$(DMSO)_2$	2.0	1.2	2.6	6.5	171.8	-164.2	-97.5
1-c5··$(DMSO)_2$	2.1	1.4	2.2	4.5	-65.7	-176.0	77.9
1-c11··$(DMSO)_2$	2.2	2.0	1.7	1.7	179.2	-63.5	98.3
1-c7··$(DMSO)_2$	2.3	1.1	1.4	8.4	-60.0	-60.9	-165.3
1-c4··$(DMSO)_2$	2.4	1.1	1.3	7.3	-61.0	-71.2	-111.7
1-c9··$(DMSO)_2$	2.4	1.9	1.2	2.0	169.4	74.4	-160.0
1-c10··$(DMSO)_2$	2.5	2.5	1.0	0.8	169.0	74.0	-97.4
1-c13··$(DMSO)_2$	2.6	2.5	0.9	0.7	169.7	-171.8	105.0
1-c19··$(DMSO)_2$	2.7	2.7	0.8	0.5	60.5	176.8	-74.2
1-c23··$(DMSO)_2$	2.8	3.5	0.6	0.1	53.0	68.2	-68.9
1-c3··$(DMSO)_2$	2.9	2.7	0.6	0.5	-64.9	-172.2	-165.9
1-c14··$(DMSO)_2$	2.9	2.4	0.5	0.8	173.0	-44.5	-96.9
1-c20··$(DMSO)_2$	3.6	4.4	0.2	0.0	61.4	170.8	-85.6
1-c18··$(DMSO)_2$	3.7	2.1	0.1	1.5	54.5	-44.8	-142.6
1-c24··$(DMSO)_2$	4.2	4.5	0.1	0.0	51.0	-48.7	93.5
1-c22··$(DMSO)_2$	4.4	4.3	0.0	0.0	55.7	55.7	-153.6
1-c12··$(DMSO)_2$	4.5	4.3	0.0	0.0	49.9	57.3	94.1
1-c21··$(DMSO)_2$	4.6	4.1	0.0	0.0	59.1	171.3	90.1

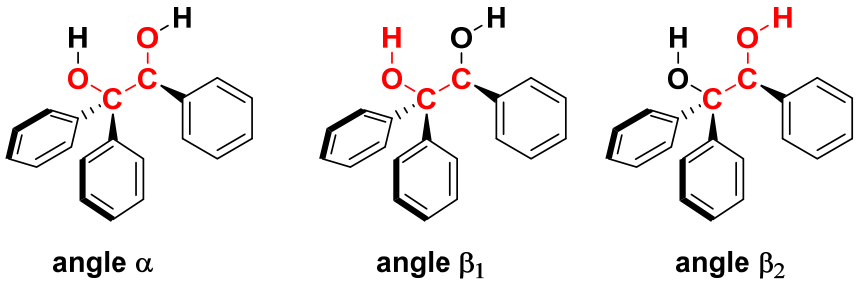
[a] referenced to E_{ZPC}= -1838.114830 hartree and G= -1838.184960 hartree

2. Conformational analysis of 2-Phenyl-1,1'-diphenyl-ethan-1,2-diol (2)

Table S8. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated (S)-2** calculated within the **IEFPCM of chloroform**.

Conf.-id	ΔE_{ZPC}[a] [kcal/mol]	ΔG_{298K}[a] [kcal/mol]	pop-ΔE_{ZPC} [%]	pop-ΔG [%]	α [deg]	β_1 [deg]	β_2 [deg]
2-c1	0.00	0.00	53.8	64.1	-57.6	53.6	166.7
2-c6	0.29	0.61	33.0	22.9	-57.4	47.3	-64.8
2-c2	1.33	1.40	5.7	6.0	-60.6	-62.0	35.9
2-c10	2.23	2.49	1.2	1.0	171.6	64.5	-57.6
2-c16	2.23	2.42	1.2	1.1	176.6	-160.1	174.5
2-c15	2.24	2.23	1.2	1.5	-178.9	-79.3	173.4
2-c7	2.57	2.63	0.7	0.8	-66.2	-52.9	178.9
2-c12	2.58	2.89	0.7	0.5	-179.0	52.0	177.7
2-c11	2.69	2.77	0.6	0.6	-174.3	-74.6	55.4
2-c17	2.72	2.78	0.5	0.6	169.0	-164.2	-61.1
2-c13	2.83	3.01	0.5	0.4	179.8	-160.8	58.0
2-c9	2.93	3.27	0.4	0.3	-175.4	46.2	54.0
2-c14	3.22	3.38	0.2	0.2	174.3	-80.4	-56.9
2-c5	3.55	3.59	0.1	0.1	-53.9	155.2	53.7
2-c8	4.48	4.85	0.0	0.0	-66.9	162.8	-55.0
2-c4	4.79	4.63	0.0	0.0	-65.9	156.3	171.4

[a] referenced to E_{ZPC}= -923.354558 hartree and G= -923.402579 hartree



Scheme S2. Angle definition for 2-phenyl-1,1'-diphenyl-ethan-1,2-diol (S)-**2**

Table S9. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated (S)-2** calculated within the **IEFPCM of acetonitrile**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
2-c1	0.00	0.00	49.8	53.6	-57.5	51.8	169.0
2-c6	0.17	0.24	37.6	35.6	-56.8	48.7	-66.4
2-c2	1.32	1.47	5.4	4.5	-59.6	-63.9	38.5
2-c7	2.03	2.19	1.6	1.3	-64.9	-54.4	-178.8
2-c15	2.24	2.14	1.1	1.4	-178.6	-74.5	179.2
2-c16	2.34	2.36	1.0	1.0	176.9	-164.4	179.0
2-c10	2.50	2.71	0.7	0.5	171.1	63.5	-58.3
2-c12	2.61	2.89	0.6	0.4	-179.2	51.3	-178.5
2-c17	2.71	4.16	0.5	0.0	169.9	-164.7	-61.2
2-c11	2.73	2.74	0.5	0.5	-174.8	-73.1	56.1
2-c13	2.97	3.16	0.3	0.3	179.7	-164.6	58.8
2-c9	3.04	3.25	0.3	0.2	-176.7	47.4	55.5
2-c14	3.09	3.38	0.3	0.2	174.9	-75.3	-58.4
2-c5	3.23	3.02	0.2	0.3	-54.7	158.1	49.7
2-c8	3.96	3.76	0.1	0.1	-65.8	162.8	-54.8
2-c4	4.57	4.36	0.0	0.0	-65.8	160.1	176.2

[a] referenced to E_{ZPC}= -923.358014 hartree and G= -923.405875 hartree

Table S10. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated (S)-2** calculated within the **IEFPCM of DMSO**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
2-c1	0.00	0.00	49.9	53.3	-57.5	51.8	169.1
2-c6	0.17	0.25	37.6	34.9	-56.8	48.8	-66.5
2-c2	1.32	1.46	5.3	4.5	-59.5	-64.0	38.6
2-c7	2.01	2.18	1.7	1.3	-64.8	-54.4	-178.6
2-c15	2.25	2.17	1.1	1.4	-178.6	-74.3	179.5
2-c16	2.36	2.38	0.9	1.0	177.0	-164.6	179.2
2-c10	2.52	2.74	0.7	0.5	171.1	63.5	-58.4
2-c12	2.62	2.89	0.6	0.4	-179.2	51.2	-178.3
2-c11	2.74	2.75	0.5	0.5	-174.9	-73.1	56.1
2-c17	2.74	2.33	0.5	1.0	170.2	-165.1	-61.1
2-c13	2.97	3.15	0.3	0.3	179.7	-164.8	58.9
2-c9	3.06	3.27	0.3	0.2	-176.7	47.4	55.6
2-c14	3.08	3.38	0.3	0.2	174.9	-75.1	-58.5
2-c5	3.22	3.04	0.2	0.3	-54.8	158.3	49.5
2-c8	3.95	3.77	0.1	0.1	-65.8	162.8	-54.8
2-c4	4.56	4.32	0.0	0.0	-65.8	160.2	176.4

[a] referenced to E_{ZPC}= -923.358177 hartree and G= -923.406039 hartree

Table S11. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **ACN-monosolvated (S)-2** calculated within the **IEFPCM of acetonitrile**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
2-c1··ACN$^{@S}$	0.00	0.00	75.2	77.1	-56.0	49.3	-176.7
2-c1··ACN$^{@T}$	1.42	1.53	6.8	5.8	-62.0	65.6	172.4
2-c10··ACN$^{@T}$	4.50	5.29	0.0	0.0	170.3	78.9	-55.5
2-c11··ACN$^{@S}$	4.41	4.32	0.0	0.1	-179.1	-72.0	86.3
2-c11··ACN$^{@T}$	3.23	4.15	0.3	0.1	-174.7	-69.3	54.1
2-c12··ACN$^{@S}$	2.87	2.62	0.6	0.9	172.8	59.3	-160.1
2-c12··ACN$^{@T}$	4.62	4.67	0.0	0.0	-179.1	65.3	179.8
2-c13··ACN$^{@S}$	4.59	5.49	0.0	0.0	175.7	-163.8	88.2
2-c13··ACN$^{@T}$	3.89	3.83	0.1	0.1	178.4	-176.1	57.9
2-c14··ACN$^{@T}$	3.61	3.81	0.2	0.1	176.5	-68.4	-56.5
2-c15··ACN$^{@S}$	2.50	2.52	1.1	1.1	-177.6	-73.2	-168.9
2-c15··ACN$^{@T}$	2.81	3.33	0.7	0.3	-177.9	-69.5	179.5
2-c16··ACN$^{@S}$	2.56	2.65	1.0	0.9	177.7	-164.7	-168.4
2-c16··ACN$^{@T}$	3.38	4.09	0.3	0.1	174.0	-170.8	179.1
2-c17··ACN$^{@T}$	3.19	3.21	0.3	0.3	168.9	-164.6	-59.9
2-c4··ACN$^{@S}$	5.08	5.29	0.0	0.0	-65.3	161.6	-168.3
2-c4··ACN$^{@T}$	5.35	6.09	0.0	0.0	-65.8	167.6	176.4
2-c5··ACN$^{@S}$	4.73	3.24	0.0	0.3	-58.4	157.6	66.7
2-c5··ACN$^{@T}$	3.44	3.80	0.2	0.1	-53.3	165.5	44.9
2-c6··ACN$^{@T}$	1.45	1.36	6.5	7.8	-61.2	62.7	-58.0
2-c7··ACN$^{@S}$	2.15	2.21	2.0	1.8	-64.4	-52.4	-168.0
2-c7··ACN$^{@T}$	4.15	3.74	0.1	0.1	-63.1	-68.5	-179.1
2-c8··ACN$^{@S}$	5.12	5.85	0.0	0.0	-65.9	158.9	-94.8
2-c8··ACN$^{@T}$	4.55	4.79	0.0	0.0	-65.3	167.4	-51.6
2-c9··ACN$^{@S}$	4.61	5.17	0.0	0.0	179.6	48.8	86.8
2-c9··ACN$^{@T}$	5.14	6.26	0.0	0.0	-177.4	64.1	59.3
2-cX_bifu	1.67	1.97	4.5	2.8	-67.0	67.7	53.5

[a] referenced to E_{ZPC}= -1056.134510 hartree and G= -1056.194590 hartree

Table S12. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **ACN twofold solvated (S)-2** calculated within the **IEFPCM of acetonitrile**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
2-c1	0.00	0.00	84.7	83.2	-61.2	64.0	-174.0
2-c15	1.33	1.12	9.0	12.6	-176.9	-68.3	-169.1
2-c16	1.90	2.45	3.4	1.3	175.5	-171.7	-168.4
2-c7	2.74	2.82	0.8	0.7	-62.7	-67.8	-167.6
2-c2	2.95	2.67	0.6	0.9	-62.4	-71.9	51.5
2-c12	3.14	3.45	0.4	0.2	-179.1	64.8	-170.8
2-c11	3.30	4.16	0.3	0.1	-178.9	-68.9	86.2
2-c10	3.60	3.44	0.2	0.2	173.4	76.8	-105.2
2-c5	3.63	3.24	0.2	0.4	-58.1	165.0	64.0
2-c13	3.87	3.66	0.1	0.2	173.8	-172.3	89.1
2-c4	4.04	4.00	0.1	0.1	-64.8	166.7	-167.9
2-c8	4.07	4.50	0.1	0.0	-65.7	165.4	-95.1
2-c9	4.95	5.78	0.0	0.0	179.0	64.5	89.1

[a] referenced to E_{ZPC}= -1188.908220 hartree and G= -1188.980290 hartree

Table S13. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **DMSO monosolvated (S)-2** calculated within the **IEFPCM of DMSO**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
2-c1··DMSO$^{@S}$	0.00	0.00	47.6	77.8	-55.2	48.3	-172.4
2-c1··DMSO$^{@T}$	1.84	3.15	2.1	0.4	-63.0	68.8	173.9
2-cX_bifu	0.00	0.83	47.4	19.1	-69.0	62.6	49.0
2-c7··DMSO$^{@S}$	2.40	2.67	0.8	0.9	-64.8	-51.6	-167.6
2-c12··DMSO$^{@S}$	2.72	3.32	0.5	0.3	-178.4	49.2	-165.3
2-c16··DMSO$^{@S}$	2.74	3.07	0.5	0.4	177.5	-165.2	-167.1
2-c15··DMSO$^{@S}$	2.84	2.88	0.4	0.6	-177.3	-71.7	-164.3
2-c17··DMSO$^{@T}$	3.44	3.95	0.1	0.1	168.9	-163.1	-59.2
2-c11··DMSO$^{@T}$	3.57	4.10	0.1	0.1	-175.7	-64.1	53.9
2-c5··DMSO$^{@T}$	3.59	4.44	0.1	0.0	-52.7	166.2	44.1
2-c16··DMSO$^{@T}$	3.61	3.42	0.1	0.2	172.1	-170.2	179.8
2-c14··DMSO$^{@T}$	3.64	4.63	0.1	0.0	176.8	-59.7	-57.3
2-c13··DMSO$^{@T}$	4.14	4.38	0.0	0.0	179.3	-178.3	56.3
2-c7··DMSO$^{@T}$	4.93	5.69	0.0	0.0	-62.9	-73.5	-179.4
2-c8··DMSO$^{@T}$	5.03	5.81	0.0	0.0	-64.6	169.4	-50.1
2-c10··DMSO$^{@T}$	5.13	6.07	0.0	0.0	170.9	81.9	-55.2
2-c4··DMSO$^{@S}$	5.18	5.46	0.0	0.0	-65.9	161.1	-166.4
2-c13··DMSO$^{@S}$	5.19	6.34	0.0	0.0	175.1	-164.7	90.5
2-c11··DMSO$^{@S}$	5.38	5.63	0.0	0.0	-179.6	-71.4	93.9
2-c5··DMSO$^{@S}$	5.52	4.62	0.0	0.0	-58.6	157.1	71.7
2-c4··DMSO$^{@T}$	5.58	6.09	0.0	0.0	-65.5	168.3	176.9
2-c9··DMSO$^{@T}$	6.03	6.45	0.0	0.0	-178.8	69.2	57.1

[a] referenced to E_{ZPC}= -1476-604840 hartree and G= -1476.667390 hartree

Table S14. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **DMSO twofold solvated (S)-2** calculated within the **IEFPCM of DMSO**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
2-c1··$(DMSO)_2$	0.00	0.20	84.9	25.7	-61.5	69.9	-166.8
2-c11··$(DMSO)_2$	3.73	1.78	0.2	1.8	179.8	-62.5	85.4
2-c12··$(DMSO)_2$	3.50	3.20	0.2	0.2	-179.6	69.5	-172.2
2-c13··$(DMSO)_2$	4.42	3.52	0.0	0.1	173.8	-171.1	103.6
2-c15··$(DMSO)_2$	1.31	0.04	9.3	33.6	-177.1	-62.9	-165.9
2-c16··$(DMSO)_2$	1.75	0.00	4.4	36.2	172.4	-163.8	-166.5
2-c2··$(DMSO)_2$	3.48	3.06	0.2	0.2	-63.6	-74.7	58.5
2-c4··$(DMSO)_2$	3.85	2.32	0.1	0.7	-64.7	168.5	-167.8
2-c5··$(DMSO)_2$	3.82	2.76	0.1	0.3	-59.2	168.6	68.4
2-c7··$(DMSO)_2$	3.22	3.05	0.4	0.2	-62.2	-72.5	-168.4
2-c8··$(DMSO)_2$	3.65	2.09	0.2	1.1	-64.6	166.3	-103.1

[a] referenced to E_{ZPC}= -2029.847140 hartree and G= -2029. 921034 hartree

3. Conformational analysis of (S,S)-hydrobenzoin (3)

Table S15. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of isolated **(S,S)-3** calculated within the **IEFPCM of acetonitrile**.

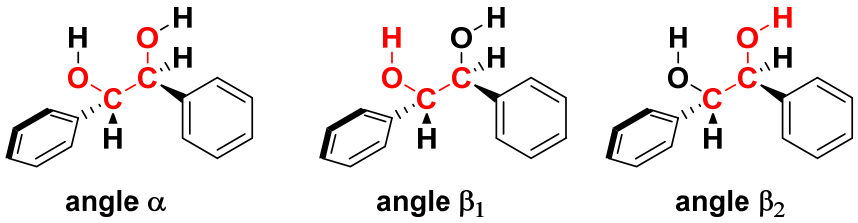
Conf.-id	ΔE_{ZPC}[a] [kcal/mol]	ΔG_{298K}[a] [kcal/mol]	pop-ΔE_{ZPC} [%]	pop-ΔG [%]	α [deg]	β_1 [deg]	β_2 [deg]
3-c1	0.0	0.0	71.0	71.9	-52.6	166.8	41.1
3-c2	0.8	0.8	18.5	18.9	-46.5	39.1	-83.9
3-c4	1.7	2.0	4.3	2.6	63.8	51.7	51.7
3-c10	1.7	1.6	3.8	4.7	54.9	-42.6	-176.0
3-c8	2.3	2.5	1.4	1.0	64.1	53.7	175.7
3-c3	2.9	2.8	0.6	0.6	-54.0	-176.4	-67.8
3-c6	3.5	3.7	0.2	0.1	-168.8	62.5	177.4
3-c5	4.0	4.0	0.1	0.1	-170.4	61.6	61.6
3-c7	4.3	4.7	0.1	0.0	-171.6	-56.6	64.3

[a] referenced to E_{ZPC}= -692.334425 hartree and G= -692.376681 hartree

Table S16. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of isolated **(S,S)-3** calculated within the **IEFPCM of DMSO**.

Conf.-id	ΔE_{ZPC}[a] [kcal/mol]	ΔG_{298K}[a] [kcal/mol]	pop-ΔE_{ZPC} [%]	pop-ΔG [%]	α [deg]	β_1 [deg]	β_2 [deg]
3-c1	0.0	0.0	70.7	71.8	-52.6	166.6	41.0
3-c2	0.8	0.8	18.8	19.2	-46.6	39.2	-83.7
3-c4	1.7	2.0	4.3	2.5	63.8	51.8	51.8
3-c10	1.7	1.6	3.8	4.5	55.0	-42.6	-176.0
3-c8	2.3	2.5	1.5	1.1	64.1	53.8	175.7
3-c3	2.8	2.8	0.6	0.6	-54.1	-176.6	-67.6
3-c6	3.5	3.7	0.2	0.1	-168.9	62.5	177.2
3-c5	4.0	3.9	0.1	0.1	-170.5	61.7	61.7
3-c7	4.3	4.7	0.1	0.0	-171.6	-56.6	64.3

[a] referenced to E_{ZPC}= -692.334425 hartree and G= -692.376681 hartree



Scheme S3. Angle definition for hydrobenzoin (S,S)-**3**

Table S17. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of mono-solvated **(S,S)-3** calculated within the **IEFPCM of ACN**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
3-c1-ACN-1	0.0	0.0	80.3	84.8	-51.1	157.9	38.5
3-c1-ACN-2	2.0	1.8	2.6	3.7	-57.6	174.3	60.8
3-c2-ACN-1	1.5	2.1	6.8	2.6	-46.8	35.5	-71.2
3-c10-ACN-2	1.8	1.7	3.7	5.1	52.8	-40.5	170.4
3-cx-ACN-bifu	2.0	2.5	2.6	1.2	-61.7	57.8	63.0
3-c8-ACN-1	2.6	3.1	1.0	0.4	63.4	51.5	163.5
3-c4-ACN-1	2.8	3.3	0.7	0.3	62.1	92.2	50.6
3-c2-ACN-2	2.9	3.3	0.6	0.3	-51.9	58.7	-78.0
3-c3-ACN-2	3.3	3.1	0.3	0.4	-54.4	171.4	-60.8
3-c8-ACN-2	3.4	3.9	0.3	0.1	62.8	99.0	178.5
3-c10-ACN-1	3.4	3.7	0.2	0.2	62.6	-55.8	-178.7
3-cx-ACN-bifu2	3.6	4.5	0.2	0.0	68.1	-54.8	-54.4
3-c6-ACN-2	3.6	3.5	0.2	0.2	-168.2	70.2	177.9
3-c3-ACN-1	3.6	4.0	0.2	0.1	-53.8	-177.3	-51.6
3-c6-ACN-1	3.8	3.8	0.1	0.1	-169.3	60.9	167.7
3-c5-ACN-1	4.1	4.2	0.1	0.1	-169.5	60.4	71.6
3-c5-ACN-2	4.2	4.3	0.1	0.1	-168.8	69.2	60.1
3-c7-ACN-1	4.2	4.3	0.1	0.1	-171.4	-55.6	72.0

[a] referenced to E_{ZPC}= -825.111247hartree and G= -825.166164hartree

Table S18. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of mono-solvated **(S,S)-3** calculated within the **IEFPCM of DMSO**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
3-c1-DMSO-2	0.0	0.0	69.1	90.0	-58.4	178.9	79.9
3-c1-DMSO-bifu	0.7	1.8	21.0	4.5	-65.5	54.8	55.5
3-c2-DMSO-2	1.5	2.0	5.3	3.0	-47.4	34.7	-66.0
3-c1-DMSO-1-bifu	2.0	4.1	2.2	0.1	68.1	-49.9	-54.5
3-c8-DMSO-1	2.7	2.9	0.7	0.7	63.2	51.4	162.9
3-c1-DMSO-1	2.9	3.1	0.5	0.4	-50.3	156.3	37.3
3-c4-DMSO-1	3.3	3.4	0.3	0.3	61.7	50.8	101.6
3-c2-DMSO-2	3.5	3.5	0.2	0.3	-53.1	73.1	-73.6
3-c3-DMSO-2	3.5	3.6	0.2	0.2	-55.0	168.4	-59.2
3-c8-DMSO-2	3.6	3.9	0.2	0.1	62.0	102.1	177.7
3-c3-DMSO-1	3.8	4.0	0.1	0.1	-54.3	-177.8	-51.2
3-c6-DMSO-2	3.9	3.9	0.1	0.1	-167.7	68.3	177.4
3-c6-DMSO-1	4.3	4.9	0.0	0.0	-169.5	60.0	162.8
3-c5-DMSO-1	4.4	4.4	0.0	0.0	-169.1	60.1	68.1
3-c5-DMSO-2	4.4	4.4	0.0	0.0	-169.1	68.1	60.1
3-c7-DMSO-1	4.5	4.9	0.0	0.0	-171.2	-55.6	67.0
3-c7-DMSO-2	6.6	7.6	0.0	0.0	-165.2	-77.4	60.8

[a] referenced to E_{ZPC}= -1245.581633 hartree and G= -1245.638755 hartree

Table S19. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of twofold solvated **(S,S)-3** calculated within the **IEFPCM of acetonitrile**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
3-c1	0.0	0.0	69.0	47.5	-56.7	163.6	55.4
3-c10	1.4	0.5	6.8	20.5	59.7	-53.8	166.8
3-c2	1.4	0.4	6.6	24.3	-52.8	49.1	-67.3
3-c8	1.5	1.8	5.6	2.4	60.9	97.0	165.2
3-c6	1.8	3.6	3.6	0.1	-168.9	70.0	167.5
3-c3	1.8	1.6	3.3	3.0	-54.6	172.4	-50.1
3-c4	1.9	2.6	2.9	0.6	59.6	93.2	93.2
3-c5	2.0	2.0	2.2	1.6	-169.1	68.0	68.0
3-c7	3.7	4.1	0.1	0.0	-166.7	-74.9	69.7

[a] referenced to E_{ZPC}= - 957.884207 hartree and G= - 957.950903 hartree

Table S20. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of twofold solvated **(S,S)-3** calculated within the **IEFPCM of DMSO**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
3-c1	0.0	0.1	71.2	25.4	-58.5	165.9	70.2
3-c10	1.6	0.8	4.6	7.1	61.3	158.5	158.8
3-c2	1.7	1.4	4.1	2.8	-55.7	170.7	-49.4
3-c6	1.9	1.8	3.0	1.4	-168.7	68.1	165.3
3-c5	1.9	0.8	2.9	7.6	-169.6	69.4	68.8
3-c3	1.9	0.9	2.9	5.7	-55.7	170.3	-51.1
3-c7	4.0	3.6	0.1	0.1	-165.5	-76.9	64.4
3-c4	1.5	0.0	5.5	27.9	60.7	104.9	158.4
3-c8	1.5	0.1	5.7	22.0	60.7	103.7	164.3

[a] referenced to E_{ZPC}= - 1798.82354 hartree and G= - 1798.893315 hartree

4. Conformational analysis of 1-Phenyl-ethan-1,2-diol (4)

Table S21. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of isolated **(S)-4** calculated within the **IEFPCM of acetonitrile**.

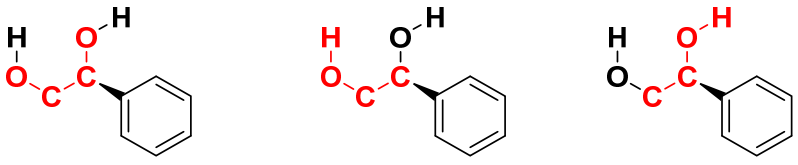
Conf.-id	ΔE_{ZPC}[a] [kcal/mol]	ΔG_{298K}[a] [kcal/mol]	pop-ΔE_{ZPC} [%]	pop-ΔG [%]	α [deg]	β_1 [deg]	β_2 [deg]
4-c1	0.0	0.0	59.4	61.7	-59.5	50.8	167.1
4-c2	0.4	0.5	32.2	28.3	-52.5	-76.6	40.5
4-c3	1.4	1.4	5.2	6.2	-62.4	-69.2	177.8
4-c4	2.3	2.4	1.3	1.1	62.5	62.4	54.7
4-c5	2.6	2.5	0.7	0.9	-177.1	69.5	59.8
4-c6	2.8	2.5	0.5	0.8	-174.0	-178.1	61.5
4-c7	2.9	2.6	0.5	0.8	-174.5	69.7	-74.5
4-c8	3.2	3.1	0.3	0.3	63.3	-179.5	52.7

[a] referenced to E_{ZPC}= -461.300385hartree and G= -461.335633 hartree

Table S22. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated (S)-4** calculated within the **IEFPCM of DMSO**.

Conf.-id	ΔE_{ZPC}[a] [kcal/mol]	ΔG_{298K}[a] [kcal/mol]	pop-ΔE_{ZPC} [%]	pop-ΔG [%]	α [deg]	β_1 [deg]	β_2 [deg]
4-c1	0.0	0.0	58.5	60.8	-59.5	50.7	167.0
4-c2	0.3	0.4	32.7	28.7	-52.5	-76.5	40.5
4-c3	1.4	1.3	5.4	6.5	-62.4	-69.3	177.7
4-c4	2.3	2.4	1.3	1.1	62.6	62.6	55.0
4-c5	2.6	2.5	0.8	0.9	-177.1	69.5	59.9
4-c6	2.8	2.5	0.6	0.9	-174.1	-178.4	61.6
4-c7	2.9	2.6	0.5	0.8	-174.6	69.7	-74.2
4-c8	3.1	3.0	0.3	0.4	63.3	-179.3	53.0

[a] referenced to E_{ZPC}= -461.335633 hartree and G= -461.33574 hartree



Scheme S4. Angle definition for 2-phenyl-1,1'-diphenyl-ethan-1,2-diol (S)-4

Table S23. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **ACN mono-solvated (S)-4** calculated within the **IEFPCM of acetonitrile**

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
4-c1$^{@S}$	0.0	0.0	44.2	32.1	-57.8	47.0	159.4
4-c2$^{@P}$	0.2	0.4	31.5	15.8	-50.8	-80.7	38.6
4-cx-bifurc	1.1	1.2	6.9	4.2	-68.7	67.1	49.5
4-c1$^{@P}$	1.1	0.6	6.4	12.6	-65.6	77.0	173.2
4-c2$^{@S}$	1.7	0.2	2.5	24.4	-59.3	-70.6	64.8
4-c3$^{@P}$	1.7	1.3	2.4	3.7	-63.2	-77.3	177.0
4-c3$^{@S}$	1.8	1.6	2.2	2.0	-63.0	-68.0	170.0
4-cx-bifurc2	2.5	2.7	0.7	0.3	69.4	-69.0	-43.5
4-c4$^{@S}$	2.5	1.9	0.6	1.2	62.9	60.6	61.9
4-c5$^{@S}$	2.7	2.1	0.5	0.9	-176.7	68.8	68.8
4-c5$^{@P}$	2.7	2.5	0.5	0.5	-176.7	78.8	58.2
4-c6$^{@P}$	2.8	2.6	0.4	0.4	-173.7	-179.0	59.2
4-c6$^{@S}$	2.9	2.4	0.3	0.6	-174.8	-179.7	69.6
4-c7$^{@P}$	3.1	2.3	0.2	0.6	-174.2	79.1	-72.4
4-c4$^{@P}$	3.1	3.1	0.2	0.2	61.7	91.9	50.7
4-c8$^{@P}$	3.3	2.9	0.2	0.2	63.7	-175.9	51.0
4-c8$^{@S}$	3.5	3.3	0.1	0.1	64.4	-176.6	63.0
4-c7$^{@S}$	3.5	3.4	0.1	0.1	-174.1	68.6	-55.1

[a] referenced to E_{ZPC}= -594.076854 hartree and G= -594.124075 hartree

Table S24. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **ACN twofold solvated (S)-4** calculated within the **IEFPCM of acetonitrile**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
4-c1	0.0	0.0	53.1	73.4	-65.3	73.2	165.9
4-c2	0.6	1.6	19.4	5.2	-59.1	-79.7	59.4
4-c3	0.7	0.9	16.8	16.4	-63.9	-76.6	167.7
4-c4	2.2	3.7	1.3	0.1	61.8	88.9	63.3
4-c5	1.5	2.1	4.0	2.1	-176.6	77.2	67.9
4-c6	1.6	2.2	3.3	1.8	-174.2	-178.1	69.1
4-c7	2.3	2.8	1.1	0.6	-173.9	76.2	-54.0
4-c8	2.4	3.2	1.0	0.3	64.7	-175.0	63.0

[a] referenced to E_{ZPC}= -726.851112 hartree and G= -726.912296 hartree

Table S25. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **DMSO mono-solvated (S)-4** calculated within the **IEFPCM of DMSO**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
4-cx-bifu	0.0	0.6	45.3	14.1	-70.1	63.2	45.5
4-c1$^{@S}$	0.3	0.0	25.7	37.8	-56.9	45.3	158.4
4-c2$^{@P}$	0.5	0.0	19.5	37.5	-50.3	-80.7	37.8
4-cx2-bifu	1.4	2.2	4.6	1.0	70.3	-65.4	-40.2
4-c1$^{@P}$	2.1	1.6	1.3	2.3	-65.9	85.9	174.8
4-c3$^{@S}$	2.2	1.9	1.1	1.6	-63.2	-66.9	165.3
4-c3$^{@P}$	2.4	1.9	0.8	1.6	-63.4	-76.3	176.9
4-c2$^{@S}$	2.6	2.7	0.6	0.4	-60.9	-69.0	77.0
4-c4$^{@S}$	3.1	2.6	0.2	0.5	63.2	60.4	60.7
4-c5$^{@S}$	3.3	2.7	0.2	0.4	-176.7	68.6	67.7
4-c5$^{@P}$	3.3	3.0	0.2	0.2	-176.5	76.0	58.0
4-c6$^{@P}$	3.5	2.8	0.1	0.3	-173.2	-175.8	57.9
4-c6$^{@S}$	3.5	2.8	0.1	0.3	-174.7	179.1	68.7
4-c7$^{@P}$	3.7	3.0	0.1	0.2	-174.5	74.9	-71.9
4-c8$^{@P}$	3.8	3.2	0.1	0.2	63.9	-177.2	50.7
4-c4$^{@P}$	3.8	3.1	0.1	0.2	61.3	95.0	50.1
4-c8$^{@S}$	3.8	2.0	0.1	1.2	64.9	-175.9	64.4
4-c7$^{@S}$	4.1	3.5	0.0	0.1	-174.5	68.1	-53.6

[a] referenced to E_{ZPC}= -1014.547637 hartree and G= -1014.595732 hartree

Table S26. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **DMSO twofold solvated (S)-4** calculated within the **IEFPCM of DMSO**.

Conf.-id	**ΔE_{ZPC}**[a] [kcal/mol]	**ΔG_{298K}**[a] [kcal/mol]	**pop-ΔE_{ZPC}** [%]	**pop-ΔG** [%]	**α** [deg]	**β_1** [deg]	**β_2** [deg]
4-c1	0.0	0.0	68.1	53.3	-65.7	77.9	164.4
4-c2	0.9	0.5	14.0	21.9	-64.4	-78.2	167.2
4-c3	1.2	1.2	8.9	6.9	-64.3	-74.2	165.3
4-c4	2.5	2.9	1.0	0.4	62.0	92.8	59.0
4-c5	1.8	1.1	3.5	7.8	-176.8	76.1	67.3
4-c6	2.0	2.1	2.4	1.5	-174.4	179.9	68.3
4-c7	2.3	1.1	1.4	7.7	-173.5	75.5	-55.1
4-c8	2.6	2.9	0.8	0.4	64.6	-174.3	62.6

[a] referenced to E_{ZPC}= -1567.790454 hartree and G= -1567.854569 hartree

5. Experimental and computed spectra

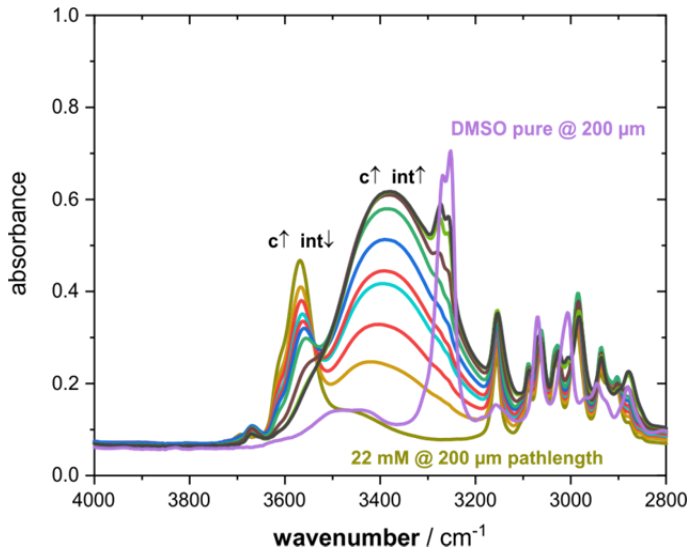


Figure S1. Titration of a 22 mM solution of **1** in $CDCl_3$ with DMSO.

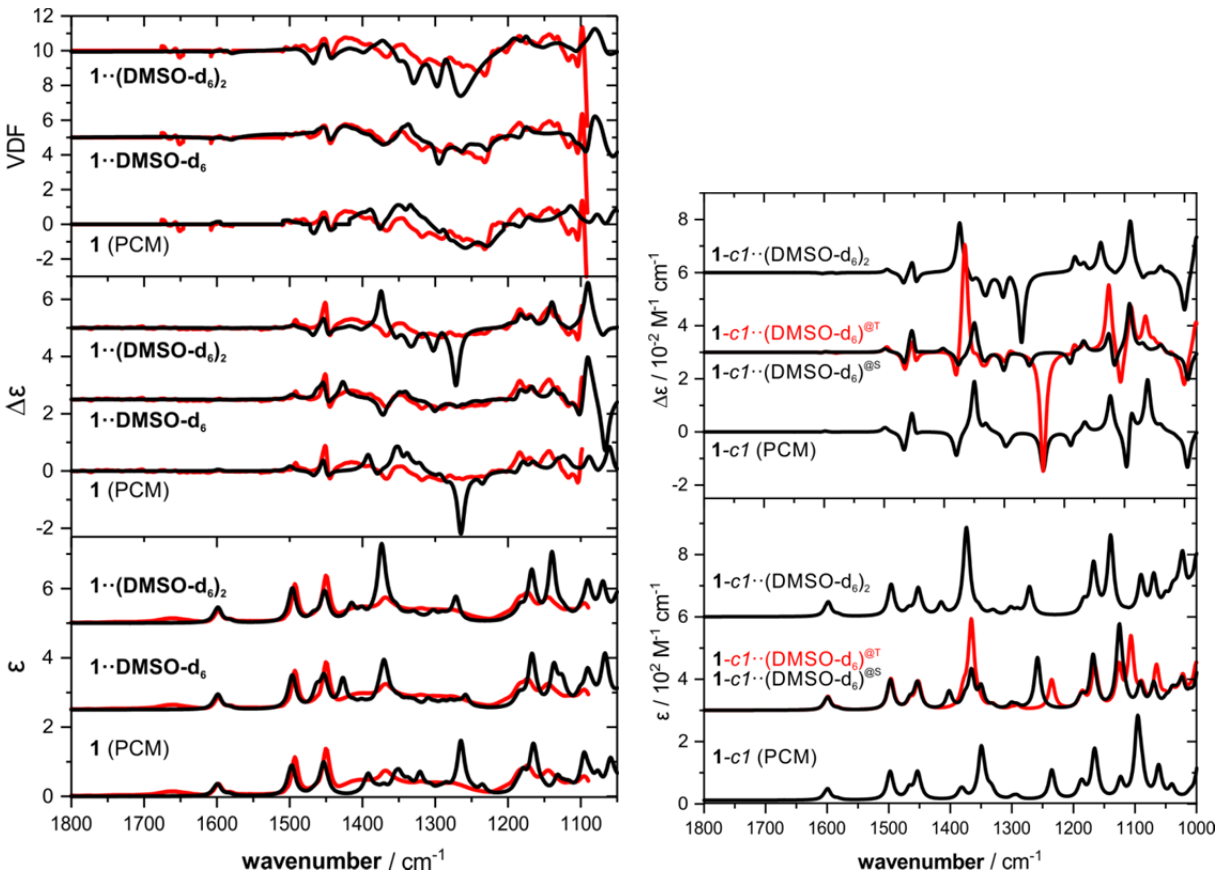


Figure S2. Left: Comparison of the experimental IR, VCD and VDF spectra of **1** in DMSO with the computed ones. Right: The computed IR and VCD spectra of **1**-c1 in different solvated forms.

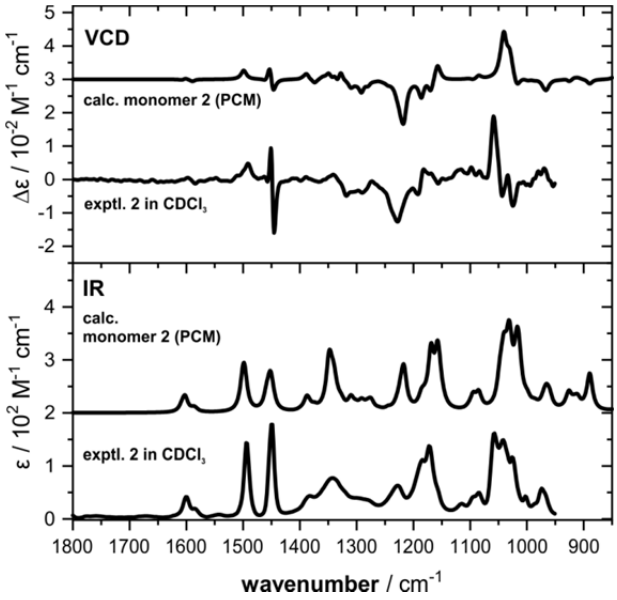


Figure S3. Comparison of the experimental IR and VCD spectra of **2** in $CDCl_3$ with the computed spectra of monomeric **2**.

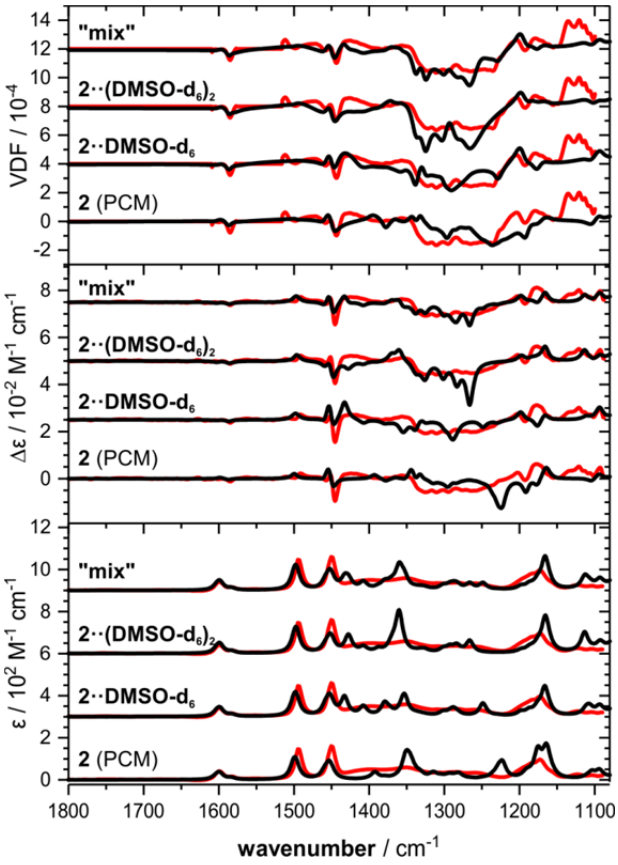


Figure S4. Comparison of the experimental IR, VCD and VDF spectra of **2** in DMSO with the computed ones.

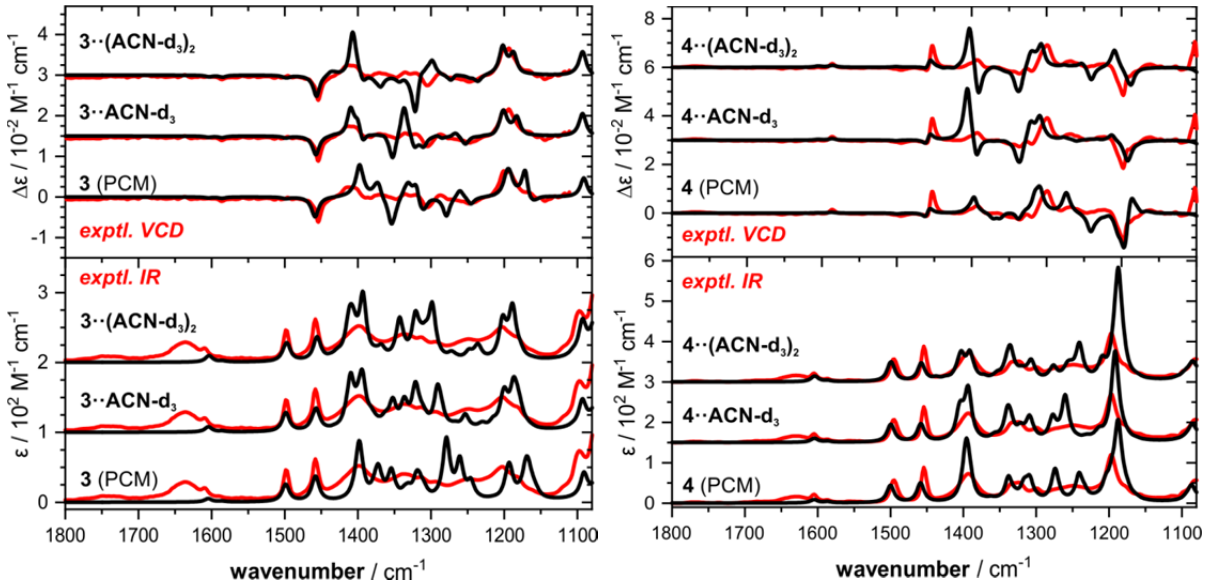


Figure S5. Comparison of the experimental IR and VCD spectra of **3** and **4** in ACN-d_3 with the computed spectra for explicitly solvated **3** and **4**.

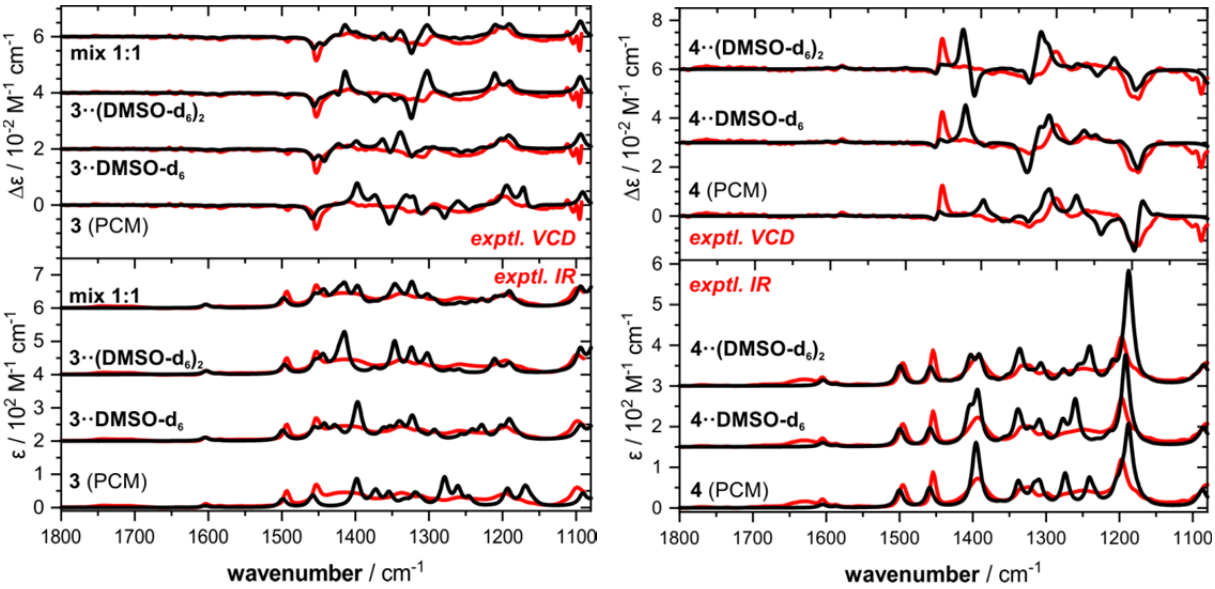


Figure S6. Comparison of the experimental IR and VCD spectra of **3** and **4** in DMSO-d_6 with the respective computed spectra.

6. Determination of frequency scaling factor

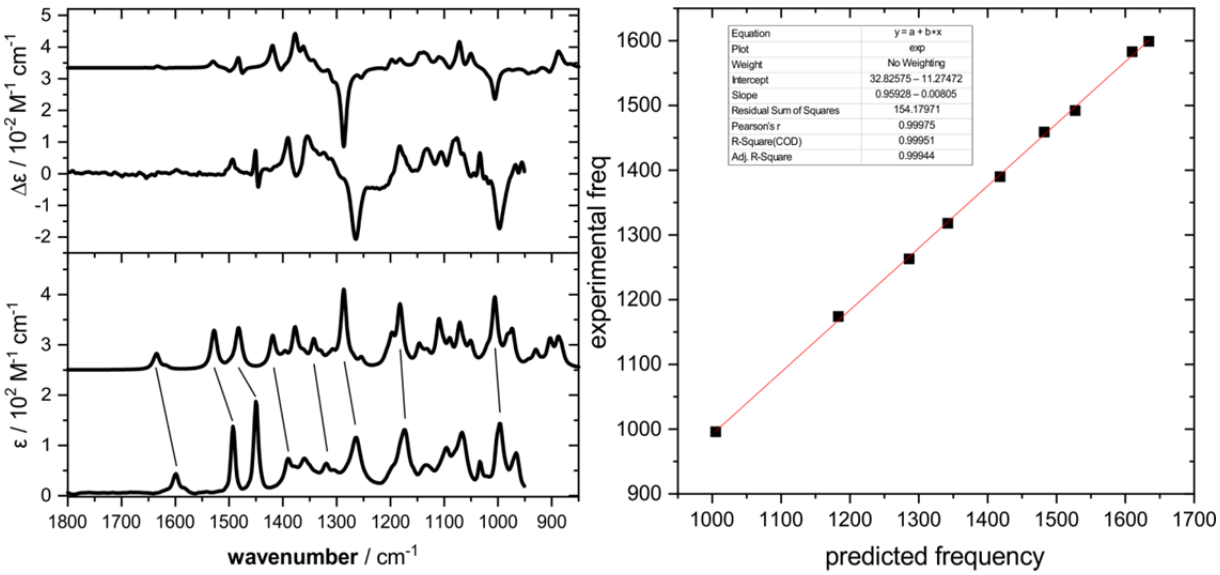


Figure S7. The assignment of experimental bands of **1** in $CDCl_3$ to the predicted and unscaled computed spectra. Based on these band assignments, we determined a linear scaling function which we employed in all calculations presented in this study.

7. Selected Cartesian coordinates

1-c1

C	-2.87211700	-1.66239600	1.06192700
C	-1.72200400	-0.89203700	1.18857200
C	-1.28821900	-0.06472500	0.14756300
C	-2.04197100	-0.03362700	-1.02674600
C	-3.19558500	-0.80491500	-1.15687600
C	-3.61633300	-1.62271300	-0.11463200
H	-3.18715700	-2.29512500	1.88363100
H	-1.15195600	-0.92671200	2.10785700
H	-1.75006800	0.59862800	-1.85435200
H	-3.76672600	-0.75875300	-2.07678100
H	-4.51412900	-2.22080700	-0.21582300
C	0.02379500	0.72564200	0.34205200
C	0.11014800	1.97422300	-0.58013200
C	1.42241100	2.73858700	-0.46678000
H	-0.02398500	1.65929400	-1.61872300
H	1.37203500	3.64186600	-1.08039900
H	1.62123000	3.02815500	0.56568200
H	2.25783000	2.14022000	-0.83059100
C	1.21589600	-0.20338000	0.09554300
C	2.19939900	-0.39018300	1.06689600
C	1.34329500	-0.87663200	-1.12319700
C	3.28554200	-1.22913100	0.82527100
H	2.11515300	0.12350500	2.01390300
C	2.43172500	-1.70620100	-1.36862500
H	0.58527600	-0.76444500	-1.88886600
C	3.40887800	-1.88781900	-0.39297200
H	4.03733500	-1.36419300	1.59425100
H	2.51251100	-2.21615500	-2.32136800
H	4.25453900	-2.53856300	-0.58093700
O	0.09692200	1.18378800	1.69507400
H	-0.52776800	1.92132600	1.75662500
O	-0.99910200	2.80189000	-0.18672400
H	-0.84585200	3.69819400	-0.50809500

1-c1..ACN

C	-2.21423300	3.30173600	0.72721100
C	-1.78538600	2.01252300	1.02260000
C	-0.88360900	1.34195500	0.19016900
C	-0.42492600	2.00344600	-0.95039800
C	-0.85238000	3.29572100	-1.24932400
C	-1.74886800	3.95137800	-0.41321100
H	-2.91332000	3.79939700	1.38942400
H	-2.14859100	1.51746900	1.91374000
H	0.28036400	1.52776600	-1.61849600
H	-0.47612200	3.78962300	-2.13767500
H	-2.07953400	4.95681600	-0.64520100
C	-0.48873700	-0.10639300	0.55321400
C	0.89575000	-0.51002700	-0.02998200
C	1.26846100	-1.96741300	0.22387800
H	0.88790200	-0.33672700	-1.11051000
H	2.28197700	-2.15085500	-0.13863100
H	1.23391500	-2.20044000	1.28896000
H	0.59660400	-2.64418400	-0.30509300
C	-1.58311200	-1.06249800	0.07108300
C	-2.23787700	-1.91760300	0.95758400
C	-1.94166800	-1.09976900	-1.27991600
C	-3.22548100	-2.79040600	0.50470600
H	-1.97200600	-1.90097200	2.00488400
C	-2.92021300	-1.97670500	-1.73429000
H	-1.46219200	-0.43566900	-1.98868500
C	-3.56904300	-2.82684600	-0.84202000
H	-3.72458100	-3.44444100	1.21040200
H	-3.17982000	-1.99124200	-2.78633600
H	-4.33564800	-3.50686400	-1.19399500
O	-0.39898100	-0.22153000	1.97664400
H	0.44582100	0.18930100	2.21451900
O	1.82888800	0.37608400	0.59649400
H	2.73896100	0.10925100	0.37384600
C	5.75672900	-0.34636000	-0.20635500
N	4.63338400	-0.19912700	-0.01318900
C	7.17764500	-0.53280000	-0.44982100
H(Iso=2)	7.70796100	0.40383100	-0.27535400
H(Iso=2)	7.56989200	-1.29667200	0.22212700
H(Iso=2)	7.33715100	-0.84757900	-1.48148700

1-c1..(ACN)$_2$

C	1.72311300	2.70357900	2.16403000
C	1.52679600	1.97282400	0.99738400
C	0.90858400	0.71864500	1.02452400
C	0.49350400	0.21724600	2.25972800
C	0.68952900	0.94627400	3.43094800
C	1.30524000	2.19230100	3.38996000
H	2.20445000	3.67358800	2.11497500
H	1.85312900	2.37924100	0.04884000
H	-0.00106300	-0.74215600	2.32558100
H	0.35256900	0.53718300	4.37644500
H	1.45539100	2.75961900	4.30087600
C	0.77175300	-0.06049400	-0.30172800
C	-0.34925400	-1.13737600	-0.25039800
C	-0.47710900	-1.94244100	-1.54093300
H	-0.12097400	-1.83016600	0.56723300
H	-1.31705900	-2.63493200	-1.45346400
H	-0.65790000	-1.28285600	-2.39032900
H	0.42166300	-2.52897200	-1.73637200
C	2.11746600	-0.72645500	-0.62147500
C	2.79366700	-0.45528100	-1.81114900
C	2.69187100	-1.62871600	0.27931400
C	4.01044000	-1.07275200	-2.09532900
H	2.36445400	0.24062400	-2.51764600
C	3.90204900	-2.25108800	-0.00591900
H	2.20005600	-1.84581400	1.21969100
C	4.56912100	-1.97495000	-1.19697600
H	4.52001000	-0.84608500	-3.02484200
H	4.32688300	-2.94838000	0.70671800
H	5.51449900	-2.45579200	-1.41864000
O	0.48730600	0.85040300	-1.36055200
H	-0.36379400	1.28742300	-1.18787900
O	-1.56164600	-0.43945000	0.03490600
H	-2.29033100	-1.08069300	0.10328800
C	-2.56008600	3.65965600	-1.70240700
N	-1.78347500	2.83041700	-1.52519100
C	-4.83175800	-2.84955200	0.53411100
N	-3.86974200	-2.24280700	0.36820100
C	-3.54283900	4.70841900	-1.92655200
H(Iso=2)	-4.54583200	4.28082000	-1.92995900
H(Iso=2)	-3.47536100	5.45413200	-1.13384100
H(Iso=2)	-3.35691800	5.19048100	-2.88677800
C	-6.04906500	-3.61595300	0.74417800
H(Iso=2)	-5.81099300	-4.67824900	0.80488200
H(Iso=2)	-6.52676300	-3.30271000	1.67288400
H(Iso=2)	-6.73700000	-3.45051500	-0.08541500

1-c1..DMSO$^{@S}$

C	3.04621100	3.20872900	-0.76707200
C	2.50202500	1.95851300	-1.03901800
C	1.62832200	1.33857800	-0.13991700
C	1.31687300	2.01102400	1.04308400
C	1.86023800	3.26443000	1.31898800
C	2.72748800	3.86960200	0.41662300
H	3.72063700	3.66718500	-1.48115700
H	2.75175500	1.45491500	-1.96380700
H	0.63815300	1.57471800	1.76345100
H	1.59740200	3.76799100	2.24206700
H	3.14848200	4.84475600	0.63093500
C	1.10099800	-0.07172400	-0.48497600
C	-0.24631400	-0.39408400	0.22365600
C	-0.73197300	-1.82335300	-0.00232000
H	-0.12408700	-0.23745900	1.30030600
H	-1.72033500	-1.94162800	0.44595600
H	-0.80528700	-2.04767400	-1.06747000
H	-0.06281800	-2.54798900	0.46315400
C	2.16967700	-1.10832000	-0.12946000
C	2.67414000	-1.98609400	-1.08905800
C	2.65601300	-1.19839100	1.17848100
C	3.63934700	-2.93244400	-0.74958100
H	2.30785700	-1.92956800	-2.10423600
C	3.61182600	-2.14837600	1.52046100
H	2.29463400	-0.51895800	1.94085000
C	4.11013700	-3.02071400	0.55565400
H	4.02078300	-3.60309400	-1.51093400
H	3.97178700	-2.20299700	2.54119900
H	4.85910100	-3.75786600	0.81962900
O	0.86394200	-0.14625500	-1.89469700
H	0.01997400	0.31026200	-2.03312300
O	-1.17411000	0.55352600	-0.30549800
H	-2.07892300	0.36817100	0.03344700
S	-4.80852500	-0.35361900	-0.23280900
O	-3.72093500	0.24769900	0.66193700
C	-5.87904200	-1.31308100	0.87530800
H(Iso=2)	-6.73873300	-1.66596400	0.30617600
H(Iso=2)	-5.29055100	-2.15863600	1.22609600
H(Iso=2)	-6.18713600	-0.68236500	1.70835800
C	-5.95880300	1.00333000	-0.59761900
H(Iso=2)	-5.42010100	1.71001700	-1.22609600
H(Iso=2)	-6.81271700	0.59695300	-1.13932700
H(Iso=2)	-6.26763500	1.47163800	0.33613500

1-c5··DMSO_bifu

C	-0.01690500	3.15572400	1.15883400
C	-0.23767700	1.78465500	1.07834700
C	-0.50247400	1.16521900	-0.14696800
C	-0.53993400	1.96375900	-1.29251500
C	-0.32072000	3.33725700	-1.21532700
C	-0.05813400	3.94081100	0.00993900
H	0.18593400	3.61078600	2.12155600
H	-0.20362800	1.18227000	1.97671200
H	-0.72645200	1.52396500	-2.26253500
H	-0.34998600	3.93377500	-2.11984900
H	0.11460500	5.00892800	0.06875500
C	-0.79794600	-0.34918800	-0.16084500
C	-0.50273800	-1.00629200	-1.55073900
C	-0.73185200	-2.51605600	-1.55599700
H	-1.17493000	-0.55515100	-2.28257200
H	-0.52841400	-2.90239200	-2.55604600
H	-0.06643400	-3.01384900	-0.84889100
H	-1.76019800	-2.76789000	-1.29315600
C	-2.27567600	-0.56578700	0.20173600
C	-2.64419100	-1.34243500	1.30104000
C	-3.28787200	0.01037500	-0.57239800
C	-3.98715300	-1.54113700	1.61581200
H	-1.87542900	-1.79521800	1.91044200
C	-4.62843400	-0.19262700	-0.26401900
H	-3.03616500	0.63403300	-1.42139800
C	-4.98574100	-0.97045700	0.83456300
H	-4.24992000	-2.14699400	2.47544900

H	-5.39452000	0.26282300	-0.88065400
H	-6.02991000	-1.12635100	1.07842000
O	-0.02282600	-0.99821500	0.84628600
H	0.92679200	-0.93112700	0.62711200
O	0.80959400	-0.69491800	-2.01857300
H	1.47589100	-0.98863600	-1.36782000
S	3.81538500	-0.25574600	0.22457000
O	2.66077100	-1.25921400	0.05595200
C	4.31248500	-0.38258800	1.96389700
H(Iso=2)	5.20753700	0.22178800	2.10941600
H(Iso=2)	3.49163300	0.01737000	2.55589700
H(Iso=2)	4.49517600	-1.42836700	2.20714700
C	5.25587800	-1.06051600	-0.52671400
H(Iso=2)	5.06241700	-1.11607600	-1.59614600
H(Iso=2)	6.13244500	-0.44176000	-0.33678100
H(Iso=2)	5.37158700	-2.05552400	-0.09936000

1-c1..(DMSO)$_2$

C	1.96435300	1.88847900	2.98436400
C	2.02164600	1.55638300	1.63522300
C	1.36473700	0.42594300	1.13842900
C	0.64801100	-0.36439400	2.03920600
C	0.58907200	-0.03571000	3.39213800
C	1.24626200	1.09168800	3.87234200
H	2.48273100	2.77066900	3.34232600
H	2.58083800	2.18272400	0.95228000
H	0.11570900	-1.24162900	1.69793600
H	0.02124600	-0.66347600	4.06923800
H	1.19838200	1.34782800	4.92416700
C	1.51931600	0.08611900	-0.36025000
C	0.38323200	-0.83976500	-0.88611900
C	0.55017300	-1.22330500	-2.35542200
H	0.39129100	-1.75864700	-0.28989700
H	-0.30891700	-1.81955900	-2.66996200
H	0.60158400	-0.33133200	-2.98089700
H	1.45080500	-1.81757200	-2.51792900
C	2.87821700	-0.60370300	-0.56099700
C	3.83996900	-0.06767300	-1.41758700
C	3.17777400	-1.79225400	0.11245100
C	5.06611800	-0.70457500	-1.60109400
H	3.62508500	0.85161000	-1.94320000
C	4.39783000	-2.43265600	-0.07396000
H	2.45960100	-2.22396500	0.79899800
C	5.35049200	-1.89062800	-0.93354800
H	5.79916500	-0.26937600	-2.27074200
H	4.60628600	-3.35377200	0.45782100
H	6.30324500	-2.38642300	-1.07707000
O	1.53598600	1.28552300	-1.12428600
H	0.71916500	1.80208200	-0.95917300
O	-0.85038200	-0.15239600	-0.68577600
H	-1.58371100	-0.80286100	-0.74182600
S	-1.86716000	3.05485500	-0.43023600
O	-0.44246400	3.24071100	-0.95158600
S	-3.56552100	-2.44592100	0.46294200
O	-2.94143800	-1.94965500	-0.84375700
C	-2.55987600	4.73089500	-0.31466800
H(Iso=2)	-3.61457200	4.65403700	-0.05076200
H(Iso=2)	-2.01444700	5.24295500	0.47595700
H(Iso=2)	-2.42746700	5.24053900	-1.26835900
C	-2.84972900	2.46911200	-1.84137200
H(Iso=2)	-2.48269500	1.47061600	-2.06840300
H(Iso=2)	-3.89754700	2.42978500	-1.54351400
H(Iso=2)	-2.70259800	3.14431800	-2.68380500
C	-5.33247500	-2.04203800	0.35386500
H(Iso=2)	-5.84144200	-2.48141700	1.21144800
H(Iso=2)	-5.40942200	-0.95708600	0.38961200
H(Iso=2)	-5.72989500	-2.42861800	-0.58385500
C	-3.70228100	-4.24841300	0.29236300
H(Iso=2)	-2.68732200	-4.64114000	0.28392700
H(Iso=2)	-4.24659300	-4.63660400	1.15299800
H(Iso=2)	-4.21626300	-4.48110900	-0.63955100

2-c1

C	3.93916100	-1.09058200	-1.26917700
C	2.56368400	-1.03266600	-1.05072600
C	2.04816400	-0.47262500	0.11809700
C	2.94887700	0.02714300	1.06474000
C	4.32008800	-0.03036400	0.85039000
C	4.82314700	-0.59025400	-0.32149800
H	4.31551800	-1.53573800	-2.18284400
H	1.90580500	-1.44648500	-1.80256900
H	2.56604600	0.46252400	1.97884500
H	4.99723100	0.36427500	1.59900600
H	5.89227900	-0.63735600	-0.49119800
C	0.54070400	-0.33451200	0.42102800
C	-0.32866100	-1.28309100	-0.46622200
H	-0.07644100	-1.08714500	-1.51213700
C	0.10594200	1.11906300	0.22210100
C	-0.61762000	1.79496100	1.20406300
C	0.41653800	1.79073200	-0.96316200
C	-1.02285600	3.11232600	1.00400100
H	-0.86329600	1.28795700	2.12613000
C	0.00393300	3.10250900	-1.16734700
H	0.99743200	1.29496100	-1.73169200
C	-0.71776600	3.77050200	-0.18204700
H	-1.58114800	3.62287400	1.78013300
H	0.25506700	3.60562900	-2.09377700
H	-1.03414400	4.79527100	-0.33660800
O	0.31187300	-0.67409000	1.78914800
H	0.48075400	-1.62384800	1.86216200
C	-1.82858500	-1.10752000	-0.32052900
C	-2.54762000	-0.45219300	-1.32205700
C	-2.52585700	-1.61882500	0.77749900
C	-3.92605700	-0.29172700	-1.22454900
H	-2.02444000	-0.06120100	-2.18739800
C	-3.90484300	-1.46388500	0.87514900
H	-1.99034800	-2.14056600	1.55917700
C	-4.60935700	-0.79668200	-0.12297800
H	-4.46537400	0.22151400	-2.01185900
H	-4.42999900	-1.86497300	1.73411100
H	-5.68352200	-0.67727200	-0.04551700
O	0.08843600	-2.60787800	-0.10708000
H	-0.54998400	-3.23853500	-0.46116400

2-c1..ACN

C	2.12624300	3.55414700	1.00023700
C	1.36574000	2.41019100	0.76496100
C	1.68824300	1.53597700	-0.27435000
C	2.79710100	1.84039400	-1.07085900
C	3.55782400	2.98058700	-0.83885200
C	3.22533100	3.84539900	0.20070300
H	1.85095800	4.21955200	1.81018400
H	0.51245200	2.22231000	1.40259800
H	3.06156900	1.17615900	-1.88324300
H	4.41212100	3.19311900	-1.47116500
H	3.81501400	4.73589400	0.38321300
C	0.92256800	0.22641000	-0.56810500
C	-0.54928300	0.27898400	-0.03955700
H	-0.51672300	0.54511500	1.02050900
C	1.68244400	-0.95576900	0.03827700
C	2.00838400	-2.07354600	-0.73004800
C	2.05694400	-0.93886500	1.38483400
C	2.69050500	-3.14920400	-0.16535200
H	1.72700700	-2.10171700	-1.77297000
C	2.72954000	-2.01561700	1.95178500
H	1.83231000	-0.07661100	2.00072400
C	3.05134500	-3.12729700	1.17737500
H	2.93764800	-4.00696500	-0.78016100
H	3.00817500	-1.98225900	2.99851400
H	3.58105100	-3.96450700	1.61617600
O	0.86775100	0.02963000	-1.98209700
H	0.24095900	0.68708500	-2.31693600
C	-1.30961600	-1.03313700	-0.15055500
C	-1.47428100	-1.83716900	0.97893300
C	-1.88389600	-1.44836600	-1.35435300
C	-2.17442900	-3.03812000	0.90762200
H	-1.05257800	-1.52110800	1.92649100
C	-2.58620000	-2.64727900	-1.42934700
H	-1.79011000	-0.82708900	-2.23487300
C	-2.73056800	-3.44916300	-0.29990900
H	-2.29146700	-3.64698300	1.79647900
H	-3.02469400	-2.95445500	-2.37177200
H	-3.28008100	-4.38126400	-0.35882900
O	-1.16631900	1.32048500	-0.79195200
H	-2.08172900	1.45151100	-0.48097500
C	-4.91383900	2.22798800	0.46092400
N	-3.86453700	1.91568100	0.11161800
C	-6.24127400	2.62246000	0.90273400
H(Iso=2)	-6.60705800	1.91570000	1.64811800
H(Iso=2)	-6.20257800	3.61918900	1.34305000
H(Iso=2)	-6.92489200	2.63261400	0.05334500

2-cx..ACN-bifu

C	-2.69815300	-2.65167300	-1.80440900
C	-1.66041400	-1.75423700	-1.56142500
C	-1.33499500	-1.37173900	-0.25860900
C	-2.07953900	-1.91453800	0.79404000
C	-3.11721100	-2.80823100	0.55411300
C	-3.43183100	-3.18247000	-0.74951700
H	-2.93440400	-2.92915600	-2.82505700
H	-1.12132800	-1.34928300	-2.40655200
H	-1.84113000	-1.63221700	1.81140900
H	-3.67879800	-3.21418800	1.38749300
H	-4.24046600	-3.87800100	-0.94018700
C	-0.16618200	-0.42689500	0.08814100
C	0.24425300	0.48386500	-1.12395000
H	0.53878700	-0.17515500	-1.94075900
C	1.04051200	-1.26218300	0.53702800
C	1.67298500	-1.02065100	1.75676900
C	1.53530200	-2.28316600	-0.27962300
C	2.77404800	-1.77916800	2.14896200
H	1.30262700	-0.23667200	2.40138300
C	2.63792100	-3.03634200	0.10738000
H	1.05411100	-2.50585700	-1.22422700
C	3.26319200	-2.78805200	1.32666300
H	3.24947100	-1.57686600	3.10180300
H	3.00416100	-3.82263800	-0.54223600
H	4.11940900	-3.37759100	1.63220900
O	-0.53513100	0.40044500	1.19224300
H	-1.35572200	0.87405000	0.98337200
C	1.42875400	1.39626400	-0.84011700
C	2.69128700	1.06795700	-1.33739900
C	1.28667500	2.58808000	-0.12472800
C	3.78903400	1.89485700	-1.11418000
H	2.81988900	0.15573500	-1.90894500
C	2.37999100	3.41882200	0.09869500
H	0.31826900	2.87872800	0.26162300
C	3.63704100	3.07397600	-0.39197400
H	4.75929900	1.62012400	-1.51118100
H	2.24923200	4.33899100	0.65627600
H	4.48748600	3.72282800	-0.21905300
O	-0.87514900	1.21092700	-1.62930900
H	-1.31482000	1.70303400	-0.91901700
C	-3.57825700	3.05009600	0.78342200
N	-2.68448200	2.38440400	0.50252400
C	-4.70796900	3.89065200	1.13931600
H(Iso=2)	-5.62795200	3.45623400	0.74724600

H(Iso=2)	-4.78069700	3.96794100	2.22455900
H(Iso=2)	-4.57247600	4.88680600	0.71710900

2-c1..DMSO

C	-2.38652700	-3.60972800	1.14138600
C	-1.70915600	-2.42322500	0.86599200
C	-2.07216700	-1.62553700	-0.22053600
C	-3.13624900	-2.05083600	-1.02275600
C	-3.81419600	-3.23372900	-0.75083200
C	-3.44175200	-4.02125000	0.33558200
H	-2.08056600	-4.21366700	1.98769800
H	-0.88727500	-2.14157300	1.51024500
H	-3.43071400	-1.44766600	-1.87163800
H	-4.63508800	-3.54022900	-1.38883200
H	-3.96668900	-4.94472400	0.54929200
C	-1.39999100	-0.27645600	-0.56204100
C	0.06239100	-0.19700200	-0.00989100
H	0.03144600	-0.42561500	1.05912300
C	-2.26122500	0.86928100	-0.02565000
C	-2.67552000	1.91061500	-0.85633900
C	-2.64630000	0.89421800	1.31795200
C	-3.45311700	2.95284700	-0.35560500
H	-2.38832800	1.90514700	-1.89799400
C	-3.41467600	1.93811900	1.82090600
H	-2.35395000	0.09024600	1.98233300
C	-3.82369700	2.97369100	0.98442600
H	-3.76756400	3.75071800	-1.01847200
H	-3.69940200	1.93830700	2.86654300
H	-4.42777500	3.78471100	1.37351300
O	-1.33011300	-0.14206700	-1.98309400
H	-0.63871800	-0.75663200	-2.26963400
C	0.71810400	1.16816700	-0.15589700
C	0.80710900	2.01904700	0.94754300
C	1.26964800	1.58977900	-1.36811700
C	1.41057900	3.26925900	0.84233300
H	0.40257700	1.70097300	1.90194800
C	1.87419600	2.83828200	-1.47767300
H	1.23493400	0.93455500	-2.22804900
C	1.94352100	3.68505600	-0.37402300
H	1.47025700	3.91351900	1.71178900
H	2.29560100	3.14937200	-2.42664800
H	2.41725400	4.65591900	-0.45953200
O	0.77213600	-1.20883700	-0.71350100
H	1.67704000	-1.30412000	-0.33354700
S	4.45241400	-0.84615200	0.00772000
O	3.21470000	-1.66351100	0.39111200
C	5.72406800	-2.06186200	-0.43972300
H(Iso=2)	5.39161600	-2.54009100	-1.35910000
H(Iso=2)	6.66187700	-1.53369500	-0.61068000
H(Iso=2)	5.82044100	-2.79056400	0.36416400
C	5.17194100	-0.28124000	1.57556000
H(Iso=2)	6.12312300	0.20643500	1.36359800
H(Iso=2)	4.47201400	0.43461600	2.00216400
H(Iso=2)	5.30357200	-1.13717500	2.23646100

2-cX..DMSO-bifu

C	1.42029100	3.29965300	-1.92023400
C	0.65168900	2.17142300	-1.64181400
C	0.47287800	1.73160900	-0.32838200
C	1.08820600	2.45575500	0.69788900
C	1.85705100	3.58153700	0.42308800
C	2.02701200	4.01033300	-0.89048900
H	1.54763800	3.61726000	-2.94863900
H	0.20713700	1.63378200	-2.46773500
H	0.96141600	2.13054100	1.72222400
H	2.32246400	4.12492800	1.23735600
H	2.62662000	4.88617500	-1.10838700
C	-0.41305300	0.52706900	0.05641500
C	-0.58327500	-0.48532100	-1.13627100
H	-1.07747700	0.05233900	-1.94639200
C	-1.79323300	1.04299700	0.49111900
C	-2.33728400	0.68963400	1.72623400
C	-2.53790700	1.87642400	-0.34896600
C	-3.59398900	1.15349800	2.11006900
H	-1.77426600	0.04902000	2.38935700
C	-3.79471800	2.33504800	0.02956400
H	-2.13593400	2.18379800	-1.30672100
C	-4.32985800	1.97559500	1.26400300
H	-3.99663600	0.86778800	3.07509300
H	-4.35346600	2.97936400	-0.63915900
H	-5.30717700	2.33593900	1.56251700
O	0.15308800	-0.14292200	1.17811000
H	1.04492200	-0.47253800	0.95156100
C	-1.46162300	-1.68269800	-0.79975800
C	-2.79199600	-1.71218000	-1.22188000
C	-0.96048100	-2.78790300	-0.10706300
C	-3.60944500	-2.80563200	-0.94685400
H	-3.19570900	-0.87191800	-1.77547300
C	-1.77289600	-3.88304000	0.16916600
H	0.07275400	-2.80157600	0.21534200
C	-3.10239800	-3.89533500	-0.24646100
H	-4.63862100	-2.80733800	-1.28663900
H	-1.36573100	-4.73070800	0.70825500
H	-3.73342400	-4.75012500	-0.03330700
O	0.67335700	-0.88845500	-1.67189000
H	1.28563600	-1.16786900	-0.96365800
S	3.90048500	-0.92115800	0.29825800
O	2.47490700	-1.49390600	0.41252400
C	4.57892400	-0.99617700	1.97777000
H(Iso=2)	5.62891500	-0.70736000	1.93578900
H(Iso=2)	4.01842300	-0.27990000	2.57530000
H(Iso=2)	4.45950200	-2.00655100	2.36633300
C	4.88397300	-2.24594000	-0.45273300
H(Iso=2)	4.52843200	-2.36029500	-1.47487400
H(Iso=2)	5.92946700	-1.93852300	-0.45235100
H(Iso=2)	4.73934500	-3.16352900	0.11567000

2-c1..DMSO$_2$

C	2.25979700	1.96158900	2.98556400
C	1.60019000	1.07093200	2.14065700
C	2.09963400	0.78422300	0.86907200
C	3.28204900	1.41581400	0.46956900
C	3.94212100	2.30619300	1.30887700
C	3.43315400	2.58414300	2.57495500
H	1.84763400	2.17066600	3.96599700
H	0.68342800	0.61519600	2.48840300
H	3.68506400	1.20713000	-0.51302400
H	4.85637000	2.78229800	0.97352600
H	3.94422600	3.27826800	3.23160700
C	1.45559900	-0.23243500	-0.09933200
C	-0.05005300	-0.49714200	0.24162900
H	-0.09289700	-0.85013900	1.27711200
C	2.24131200	-1.55078200	-0.01613500
C	2.76875500	-2.14791400	-1.16114900
C	2.44129200	-2.18286500	1.21482000
C	3.47278000	-3.34779400	-1.07927700
H	2.62729600	-1.66985300	-2.11968200
C	3.13847700	-3.38300600	1.29823100
H	2.06043400	-1.73416900	2.12428200
C	3.65906100	-3.97262500	0.14888200
H	3.87543100	-3.79349000	-1.98168100
H	3.28034700	-3.85438000	2.26380600
H	4.20681300	-4.90542300	0.21242600
O	1.56382100	0.24066900	-1.43314600
H	1.19828000	1.14617900	-1.51002500
C	-0.69938100	-1.56964100	-0.62068500
C	-0.89920900	-2.85463800	-0.11290300
C	-1.14289500	-1.28928500	-1.91547600
C	-1.50740400	-3.84378200	-0.88168500
H	-0.57821400	-3.08650200	0.89654000
C	-1.75260200	-2.27378800	-2.68674600
H	-1.01347300	-0.29284600	-2.31481100
C	-1.93424800	-3.55666800	-2.17447700
H	-1.65392600	-4.83450100	-0.46719400
H	-2.08918600	-2.03883700	-3.69010700
H	-2.41170600	-4.32213000	-2.77495800
O	-0.72603300	0.74866700	0.12560500
H	-1.61669100	0.66255400	0.53374700
S	-0.01414800	3.95429400	-2.00843900
O	0.98114000	2.83449600	-2.31018500
S	-4.19251200	-0.43005900	1.26046400
O	-3.18651500	0.72013000	1.35370500
C	-0.03421800	4.14845500	-0.20136300
H(Iso=2)	0.93515000	4.55563600	0.08041200
H(Iso=2)	-0.82399600	4.85316000	0.05884800
H(Iso=2)	-0.19754100	3.17096700	0.25073300
C	-1.67081900	3.23150600	-2.20269000
H(Iso=2)	-2.40857600	3.97147900	-1.89216700
H(Iso=2)	-1.79208100	3.00689000	-3.26099400
H(Iso=2)	-1.72754600	2.32709900	-1.59857600
C	-5.73827000	0.31015800	0.66065600
H(Iso=2)	-5.55776000	0.62527200	-0.36530900
H(Iso=2)	-6.51795300	-0.45088500	0.68593400
H(Iso=2)	-5.99530400	1.16220800	1.28878900
C	-4.71157100	-0.76582100	2.96774100
H(Iso=2)	-5.51921200	-1.49720700	2.94765500
H(Iso=2)	-3.84653200	-1.17878800	3.48325200
H(Iso=2)	-5.03191000	0.16575600	3.43280900

2-c1..ACN$_2$

C	-1.92142400	2.34377500	-2.89065700
C	-1.25575800	1.38360200	-2.13110000
C	-1.61865400	1.13973600	-0.80527300
C	-2.66966300	1.88641000	-0.26276200
C	-3.33527100	2.84592500	-1.01730200
C	-2.96385800	3.07971700	-2.33878300
H	-1.61626500	2.51759300	-3.91604000
H	-0.44094100	0.83973000	-2.58895300
H	-2.96490300	1.71271900	0.76387400
H	-4.14623800	3.41070700	-0.57202400
H	-3.47946500	3.82762200	-2.92945800
C	-0.96349700	0.05648300	0.08050600
C	0.46535500	-0.33099800	-0.42619900
H	0.36585600	-0.67267300	-1.46152100
C	-1.86624800	-1.18463800	0.09683800
C	-2.30247900	-1.74177800	1.29895400
C	-2.26731000	-1.78611600	-1.09966800
C	-3.11651400	-2.87275600	1.30526500
H	-2.00357700	-1.28783100	2.23270800
C	-3.07385500	-2.91869900	-1.09521700
H	-1.95910700	-1.36601600	-2.04937700
C	-3.50397300	-3.46811700	0.10998300
H	-3.44611700	-3.28818500	2.25066900
H	-3.37146700	-3.36828200	-2.03535300
H	-4.13684800	-4.34765900	0.11527300
O	-0.87151800	0.53017700	1.41798700
H	-0.34462900	1.34754800	1.43964200
C	1.11900600	-1.45886800	0.35730400
C	1.15852700	-2.74931800	-0.17386600
C	1.72316000	-1.22884100	1.59591700
C	1.76640400	-3.79213600	0.52030100
H	0.71146500	-2.94262500	-1.14260400
C	2.33300200	-2.26768800	2.29212200
H	1.72101600	-0.23026800	2.01092800
C	2.35374000	-3.55461200	1.75910700
H	1.78709800	-4.78640000	0.08941000
H	2.79590700	-2.07175000	3.25253400
H	2.83142600	-4.36244300	2.30098500
O	1.23865500	0.86299300	-0.37751900
H	2.11174500	0.69097500	-0.77427300

C	0.77635400	4.10400900	2.69779200
N	0.35528400	3.11529700	2.28910400
C	4.88365000	0.36750700	-2.14639700
N	3.85677700	0.49802500	-1.64701000
C	1.31073100	5.35486400	3.21273000
H(Iso=2)	0.78297300	5.63568600	4.12454600
H(Iso=2)	2.37190500	5.23958100	3.43530300
H(Iso=2)	1.18537000	6.14356700	2.47028300
C	6.18279800	0.20032400	-2.77697700
H(Iso=2)	6.43868200	-0.85879900	-2.81847600
H(Iso=2)	6.15624700	0.60211600	-3.79028100
H(Iso=2)	6.94300500	0.72976500	-2.20191000

3-c1

C	2.40859600	-1.82157500	1.09524400
C	1.56307900	-0.72696200	1.25689300
C	1.52141400	0.28859900	0.30128700
C	2.35227000	0.19519100	-0.81876700
C	3.19965000	-0.89529100	-0.98112700
C	3.22853100	-1.90879500	-0.02536900
H	2.43005800	-2.60145700	1.84722700
H	0.93079700	-0.66187100	2.13546600
H	2.34438200	0.98518200	-1.56005500
H	3.83956300	-0.95438800	-1.85371300
H	3.89007100	-2.75753500	-0.15188000
C	0.59021100	1.46792600	0.47909900
H	0.18794700	1.46277800	1.49703700
C	-0.60233100	1.47201600	-0.50262800
H	-0.19173400	1.44073700	-1.51895800
O	-1.34617100	2.68142000	-0.32866000
H	-0.69024900	3.38534100	-0.21615300
O	1.25481600	2.72176900	0.23732300
H	1.88330900	2.88371900	0.95122300
C	-1.53208400	0.29583900	-0.31311000
C	-1.55149900	-0.74638200	-1.23947200
C	-2.38365200	0.23112800	0.79263500
C	-2.39519100	-1.84010500	-1.06220400
H	-0.90394200	-0.70300600	-2.10797400
C	-3.23085200	-0.85744000	0.96977700
H	-2.39121700	1.04183200	1.51086500
C	-3.23709900	-1.89846800	0.04383700
H	-2.39852000	-2.64145200	-1.79157500
H	-3.88804200	-0.89338800	1.83073800
H	-3.89783000	-2.74608700	0.18188400

3-c1-ACN

C	-0.15335900	2.81595500	1.31355900
C	-0.21393100	1.44756300	1.06144900
C	-0.37110700	0.96747700	-0.23894300
C	-0.47666400	1.88619700	-1.28663900
C	-0.41855200	3.25334500	-1.03827900
C	-0.25429000	3.72293900	0.26333600
H	-0.03312000	3.17183000	2.33006400
H	-0.14065800	0.74647700	1.88556000
H	-0.61820600	1.52877300	-2.29947200
H	-0.50332600	3.95404500	-1.86073900
H	-0.21111000	4.78822200	0.45676700
C	-0.42054400	-0.52298700	-0.50715200
H	-0.54605700	-1.05381400	0.44263600
C	0.86144400	-1.06413200	-1.18323600
H	1.01704400	-0.48500700	-2.10171200
O	0.65739800	-2.43916900	-1.52056100
H	-0.26321300	-2.49366100	-1.82170000
O	-1.48441600	-0.87973300	-1.39666900
H	-2.32374800	-0.89487100	-0.89928900
C	-5.01479100	-1.07714300	0.56812500
N	-3.99485100	-1.01306700	0.04270000
C	-6.30529600	-1.15773000	1.23190300
H(Iso=2)	-6.94456600	-0.34106000	0.89532300
H(Iso=2)	-6.78355800	-2.10829500	0.99400700
H(Iso=2)	-6.17016600	-1.08510800	2.31141900
C	2.09364200	-0.94607700	-0.31679400
C	3.08375400	-0.01152000	-0.61894400
C	2.26122500	-1.76620200	0.80210400
C	4.21433500	0.11364200	0.18479500
H	2.97185500	0.62327300	-1.49080900
C	3.39114600	-1.64724300	1.60398400
H	1.50858100	-2.50824400	1.03925100
C	4.37066600	-0.70422700	1.29921000
H	4.97416400	0.84493600	-0.06441700
H	3.50882200	-2.29168400	2.46733600
H	5.25129900	-0.61229900	1.92384000

4-c1

C	-2.44936300	1.14876300	0.18379800
C	-1.08097000	1.19947600	0.43463500
C	-0.27658500	0.07761300	0.22797300
C	-0.86813200	-1.10229900	-0.22948400
C	-2.23636200	-1.15663300	-0.47635700
C	-3.03064600	-0.03060400	-0.27289700
H	-3.06117400	2.02718500	0.35201000
H	-0.63469800	2.11879400	0.79879000
H	-0.25569200	-1.98289300	-0.38019300
H	-2.68346400	-2.07918300	-0.82775900
H	-4.09631700	-0.07417300	-0.46385500
C	1.21734300	0.16301300	0.46150700
H	1.43311100	1.01962400	1.10878100
C	1.98449100	0.34838900	-0.84482600
H	1.65141300	1.25880000	-1.34293200
H	1.78017800	-0.50343300	-1.50484000
O	3.38499800	0.48606400	-0.62031400
H	3.65088200	-0.25138500	-0.05459700
O	1.76378200	-1.02759500	1.05056900
H	1.46687500	-1.08739800	1.96645700

3-c1-(ACN)$_2$

C	-2.40035400	3.05088400	0.16324200
C	-1.60292700	2.03408200	-0.35636600
C	-0.78594900	1.26931600	0.47682300
C	-0.77460600	1.54994300	1.84592200
C	-1.56939400	2.56468700	2.36867500
C	-2.38709900	3.31796300	1.52874600
H	-3.02667500	3.63663600	-0.49945600
H	-1.61496600	1.83494700	-1.42234300
H	-0.13020700	0.97879500	2.50329700
H	-1.54934700	2.77031700	3.43267700
H	-3.00408300	4.11035900	1.93572000
C	0.07156500	0.15499700	-0.09348300
H	0.08743500	0.24186400	-1.18596200
C	-0.45660500	-1.25672200	0.25245500
H	-0.46047200	-1.34085400	1.34632300
O	0.40275900	-2.25057900	-0.30191700
H	1.30974100	-2.09564400	0.01117500
O	1.40594000	0.19503000	0.41311800
H	1.87664300	0.94489800	0.00651500
C	3.58645100	3.21995700	-1.22073100
N	2.92435400	2.37932400	-0.80147700
C	4.33236200	-3.28088100	0.66388800
N	3.28107200	-2.87200000	0.43993100
C	4.42464100	4.28351500	-1.74929800
H(Iso=2)	5.10927900	4.63217300	-0.97559500
H(Iso=2)	5.00149000	3.91234200	-2.59684500
H(Iso=2)	3.80162600	5.11604900	-2.07736600
C	5.66248300	-3.79711300	0.94699200
H(Iso=2)	6.23690500	-3.86608500	0.02276800
H(Iso=2)	6.17831500	-3.13062300	1.63882000
H(Iso=2)	5.58745500	-4.78822800	1.39524300
C	-1.85807800	-1.50838700	-0.25843600
C	-2.93465300	-1.57468700	0.62553800
C	-2.09911800	-1.68076300	-1.62412400
C	-4.22811900	-1.79757400	0.15933900
H	-2.76154700	-1.45264100	1.68892300
C	-3.38880200	-1.90744100	-2.09309000
H	-1.27181200	-1.64766400	-2.32251200
C	-4.45877200	-1.96413100	-1.20245400
H	-5.05256200	-1.84669700	0.86094500
H	-3.55963000	-2.04118500	-3.15496600
H	-5.46332200	-2.14151000	-1.56798000

3-c1-(DMSO)$_2$

C	-2.21045500	3.28074300	0.48624900
C	-1.73912400	2.16291800	-0.19821900
C	-1.05063500	1.15061200	0.47126600
C	-0.83280100	1.28595200	1.84526100
C	-1.30263500	2.39988700	2.53312200
C	-1.99527500	3.40148900	1.85572400
H	-2.74062100	4.05823600	-0.05147600
H	-1.90761100	2.07778400	-1.26619100
H	-0.28206800	0.51870700	2.37607100
H	-1.12612700	2.48882900	3.59890400
H	-2.35856100	4.27096200	2.39079500
C	-0.54802300	-0.07198600	-0.27643100
H	-0.63327100	0.11474300	-1.35377600
C	-1.36770200	-1.34945400	0.03248600
H	-1.25824100	-1.55109300	1.10518100
O	-0.87367500	-2.45277000	-0.71851300
H	0.00574200	-2.71971000	-0.37491600
O	0.80423700	-0.37478200	0.05546500
H	1.38578700	0.31669300	-0.33201500
S	2.80840000	-3.04107300	0.01863000
O	1.43607600	-3.69509900	0.18836800
C	3.19108600	-2.24807000	1.60682000
H(Iso=2)	4.21354500	-1.87232300	1.56845600
H(Iso=2)	2.48677300	-1.42526300	1.70768700
H(Iso=2)	3.06741100	-2.97582500	2.40819400
C	4.00671800	-4.40304400	0.11696400
H(Iso=2)	3.86035900	-5.01722900	-0.76962200
H(Iso=2)	5.01133300	-3.98044200	0.11689700
H(Iso=2)	3.82089700	-4.98006100	1.02215300
S	2.76434900	2.80792100	-0.45173000
O	2.50071400	1.45136800	-1.11039700
C	2.49413800	4.04821900	-1.74986300
H(Iso=2)	1.43082200	4.03341500	-1.98124700
H(Iso=2)	2.77812000	5.02532900	-1.35952800
H(Iso=2)	3.08565000	3.78354900	-2.62552700
C	4.57007700	2.95361400	-0.32708100
H(Iso=2)	4.81280300	3.95387400	0.03096700
H(Iso=2)	4.89618400	2.20875600	0.39635300
H(Iso=2)	5.01187200	2.76473600	-1.30471700
C	-2.84052600	-1.18883200	-0.28101000
C	-3.78159800	-1.08971500	0.74343300
C	-3.28480300	-1.14378600	-1.60535600
C	-5.13646400	-0.93851500	0.45692900
H	-3.45387500	-1.13230100	1.77615700
C	-4.63708300	-0.99632200	-1.89590200
H	-2.56925300	-1.23533500	-2.41348100
C	-5.56820900	-0.89040100	-0.86475100
H	-5.85321800	-0.86412500	1.26641800
H	-4.96558600	-0.96491000	-2.92833500
H	-6.62177500	-0.77615100	-1.09102100

4-c1..ACN

C	2.27512600	-1.98467400	-1.15548500
C	1.55702300	-0.79634400	-1.25635700
C	1.15431300	-0.10617200	-0.11157500
C	1.48053100	-0.63105200	1.14055700
C	2.19527300	-1.82077200	1.24448600

C	2.59656300	-2.50047800	0.09696000
H	2.57650800	-2.51047700	-2.05391000
H	1.30162500	-0.40474400	-2.23549300
H	1.16050200	-0.11058900	2.03478300
H	2.43832900	-2.21869400	2.22291700
H	3.15072200	-3.42804800	0.17847000
C	0.41385200	1.21138700	-0.24029600
H	-0.08185900	1.24730500	-1.21725400
C	1.37286200	2.39775200	-0.15377700
H	2.11205300	2.34341200	-0.95318300
H	1.89795500	2.36288500	0.80894500
O	0.68230800	3.63583700	-0.30276700
H	-0.08994100	3.58345700	0.27796800
O	-0.55064000	1.42282200	0.79199600
H	-1.35223500	0.90546500	0.59196200
C	-3.96616500	-0.62483900	0.00625900
N	-2.99519300	-0.04514300	0.21076000
C	-5.19363600	-1.35916800	-0.25246700
H(Iso=2)	-5.47227500	-1.93448800	0.63085900
H(Iso=2)	-5.99680700	-0.66245800	-0.49391300
H(Iso=2)	-5.04602300	-2.04014600	-1.09113900

4-c1..(ACN)$_2$

C	-4.03050000	-1.28779300	-0.50120100
C	-2.74903900	-1.04531900	-0.98813000
C	-1.66414700	-0.92338100	-0.11763500
C	-1.88849600	-1.04506300	1.25537700
C	-3.16887800	-1.28543000	1.74578700
C	-4.24404900	-1.40917800	0.86919900
H	-4.86201400	-1.37476300	-1.19087000
H	-2.59135800	-0.94382000	-2.05691500
H	-1.05681500	-0.93834400	1.94092000
H	-3.32779900	-1.37494600	2.81425200
H	-5.24112000	-1.59326500	1.25150500
C	-0.26476700	-0.70884600	-0.66800900
H	-0.34350100	-0.27388500	-1.67180200
C	0.47336500	-2.04271400	-0.79961500
H	-0.14597600	-2.73610100	-1.37105900
H	0.62008100	-2.46516000	0.20219100
O	1.70853800	-1.93193400	-1.49129000
H	2.36316100	-1.49375400	-0.92175500
O	0.53719000	0.13101100	0.15870700
H	0.21790100	1.04758200	0.08188900
C	-0.63746300	4.03301000	-0.15252300
N	-0.32053100	2.93087700	-0.07612100
C	5.09321800	-0.53031500	0.37477700
N	4.10291700	-0.91698700	-0.06263100
C	-1.03873200	5.42692500	-0.24941300
H(Iso=2)	-0.80279400	5.94455300	0.68083700
H(Iso=2)	-0.50725200	5.90763700	-1.07117700
H(Iso=2)	-2.11187700	5.49004100	-0.43167300
C	6.34549300	-0.03911500	0.92702100
H(Iso=2)	6.44851600	1.02593200	0.71734500
H(Iso=2)	6.35963000	-0.19382900	2.00624200
H(Iso=2)	7.18265900	-0.57441900	0.47819700