Supporting information for

Solvation and self-aggregation of chiral alcohols: How hydrogen bonding affects their VCD spectral signatures

Luisa Weirich,[a] Christian Merten*[a]

Ruhr Universität Bochum, Lehrstuhl für Organische Chemie II
Universitätsstraße 150, 44801 Bochum, Germany

Contents

1. Conformational analysis of 1-Phenyl propanol (1PP)

1.1 Monomeric 1PP

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

Conf.	**α** (C_{Ar}-C*-O-H)	**β** (C_{Ar}-C*-CH_2-CH_3)	**ΔE_{ZPC}[a] [kcal/mol]**	**ΔG_{298K}[a] [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**
1PP-c1 (8)	-57.1	174.5	0.00	0.00	41.4	40.9
1PP-c2 (5)	-52.5	64.4	0.28	0.37	25.6	21.9
1PP-c3 (4)	-58.1	-62.9	1.21	1.32	5.4	4.4
1PP-c4 (1)	179.5	176.4	0.82	0.59	10.4	15.0
1PP-c5 (2)	174.1	64.8	1.14	1.19	6.0	5.5
1PP-c6 (3)	179.6	-61.5	1.71	1.74	2.3	2.2
1PP-c7 (7)	60.3	173.4	1.35	1.27	4.2	4.8
1PP-c8 (6)	61.0	63.0	1.41	1.32	3.9	4.4
1PP-c9 (9)	76.9	-63.6	2.28	2.27	0.9	0.9

[a] referenced to E=-425.355158 hartree and G=-425.387098 hartree

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

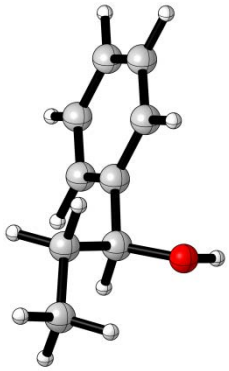
Conf.	**α** (C_{Ar}-C*-O-H)	**β** (C_{Ar}-C*-CH_2-CH_3)	**ΔE_{ZPC}[a] [kcal/mol]**	**ΔG_{298K}[a] [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**
1PP-c1	-58.2	174.2	0.00	0.00	35.8	26.2
1PP-c2	-54.3	64.2	0.24	0.34	23.9	14.8
1PP-c3	-59.3	-62.7	1.22	1.39	4.5	2.5
1PP-c4	-178.7	176.2	0.68	0.57	11.5	10.0
1PP-c5	175.5	64.8	0.80	0.86	9.2	6.2
1PP-c6	179.0	-61.6	1.60	1.77	2.4	1.3
1PP-c7	75.7	173.6	1.06	0.97	6.0	5.1
1PP-c8	66.8	62.6	1.10	0.77	5.6	7.1
1PP-c9	77.0	-63.6	2.09	2.15	1.1	0.7

[a] referenced to E= -425.356930 hartree and G= -425.392557 hartree

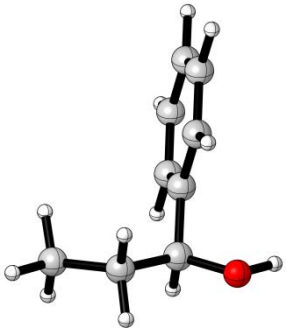
Table S3. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated 1PP** calculated within the **IEFPCM of DMSO**.

Conf.	**α** (C_{Ar}-C*-O-H)	**β** (C_{Ar}-C*-CH_2-CH_3)	**ΔE_{ZPC}[a] [kcal/mol]**	**ΔG_{298K}[a] [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**
1PP-c1	-58.2	174.2	0.00	0.00	35.6	35.1
1PP-c2	-54.4	64.2	0.24	0.33	23.8	19.9
1PP-c3	-59.4	-62.7	1.22	1.39	4.5	3.3
1PP-c4	-178.6	176.2	0.67	0.55	11.5	13.8
1PP-c5	175.6	64.8	0.79	0.84	9.4	8.5
1PP-c6	179.0	-61.6	1.60	1.77	2.4	1.8
1PP-c7	75.9	173.6	1.05	1.00	6.0	6.5
1PP-c8	67.1	62.6	1.08	0.73	5.7	10.1
1PP-c9	77.0	-63.6	2.08	2.14	1.1	0.9

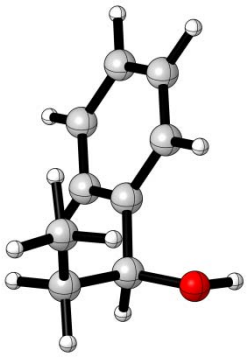
[a] referenced to E= -425.357006 hartree and G= -425.392636 hartree



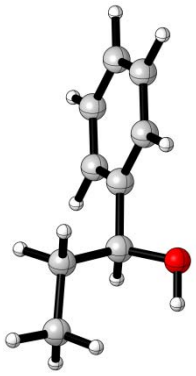
1PP-c1



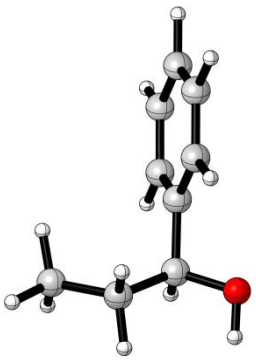
1PP-c2



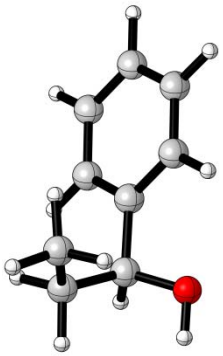
1PP-c3



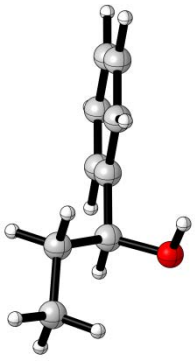
1PP-c4



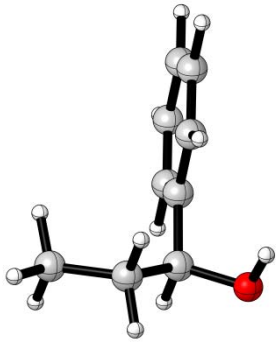
1PP-c5



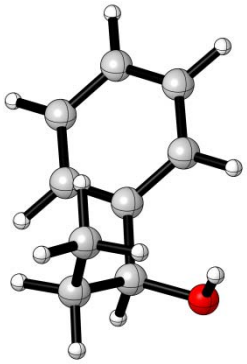
1PP-c6



1PP-c7



1PP-c8



1PP-c9

Figure S1. The nine unique conformations of monomeric 1PP

1.2 Explicit solvation of 1PP

Table S4. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **1PP mono-solvated** with **DMSO-d_6** calculated within the **IEFPCM of DMSO**.

Conf.	**$\Delta E^{[a]}$ [kcal/mol]**	**$\Delta G^{[a]}$ [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**	**α** (C_{Ar}-C*-O-H)	**β** (C_{Ar}-C*-CH_2-CH_3)	**δ_1** (C*-O··O=S)	**δ_2** (O··O=S-CH_3)
1PP-c1	0.00	0.00	7.1	12.3	-89.8	173.3	-103.7	-127.5
	0.01	0.53	7.0	5.0	-49.7	173.4	97.5	-136.1
	0.06	0.14	6.3	9.6	-68.6	173.5	-179.3	-129.6
	0.13	0.33	5.7	7.1	-76.3	173.3	-26.8	-123.1
	0.17	0.10	5.3	10.3	-82.8	173.5	-113.7	58.9
	0.25	0.60	4.6	4.5	-78.0	173.2	-152.9	50.3
	0.40	1.31	3.6	1.3	-62.3	172.7	65.0	37.5
1PP-c2	0.36	0.93	3.9	2.5	-45.5	63.2	114.4	-127.7
	0.39	0.99	3.7	2.3	-84.8	63.2	-120.2	-129.3
	0.39	0.99	3.6	2.3	-87.0	63.0	-102.3	-128.2
	0.47	0.99	3.2	2.3	-70.8	63.1	-26.3	-125.1
	0.57	1.46	2.7	1.0	-80.0	63.1	-123.6	55.8
	0.59	1.32	2.6	1.3	-69.8	63.1	-167.4	48.8
	0.60	0.99	2.6	2.3	-52.4	62.9	116.0	41.3
	0.88	2.19	1.6	0.3	-64.4	63.1	8.6	53.5
1PP-c3	1.12	1.60	1.1	0.8	-53.7	-64.2	89.9	-131.0
	1.13	1.60	1.1	0.8	-91.3	-64.1	-90.4	-125.1
	1.17	1.64	1.0	0.8	-50.8	-64.2	119.0	-133.3
	1.29	2.29	0.8	0.3	-67.9	-64.1	13.4	-127.1
	1.33	1.47	0.7	1.0	-82.3	-64.2	-147.3	50.4
	1.38	2.08	0.7	0.4	-87.9	-64.3	-113.7	52.0
	1.52	2.04	0.5	0.4	-64.5	-64.5	68.9	46.6
	1.54	2.56	0.5	0.2	-62.9	-64.4	94.1	43.1
1PP-c4	0.03	0.47	6.7	5.6	-89.9	173.3	-101.1	137.6
	0.81	0.98	1.8	2.4	-119.7	174.7	111.4	118.8
1PP-c5	0.88	1.12	1.6	1.8	-150.9	64.5	111.9	129.9
	0.89	1.09	1.6	1.9	-151.3	64.6	94.5	120.4
	0.89	1.26	1.6	1.5	170.9	64.5	-101.7	137.8
	0.90	1.52	1.6	0.9	-155.1	64.6	132.1	130.0
	0.96	1.29	1.4	1.4	-170.1	64.5	175.6	130.3
	1.02	1.17	1.3	1.7	-159.0	64.6	137.8	51.0
	1.09	0.93	1.1	2.5	-176.4	64.6	-159.7	59.5
1PP-c6	1.36	1.12	0.7	1.9	-150.6	-62.4	121.0	-134.3
	1.40	1.42	0.7	1.1	-149.9	-62.3	114.4	-131.9
	1.52	1.99	0.5	0.4	176.8	-62.4	-90.2	-125.2
	1.53	2.01	0.5	0.4	172.4	-62.5	-111.2	-126.4
	1.59	1.90	0.5	0.5	-168.2	-62.9	0.2	-136.2
1PP-c7	1.12	1.29	1.1	1.4	96.1	173.4	123.1	-135.8
	1.18	1.87	1.0	0.5	69.6	173.1	-167.3	-125.3
	1.19	1.58	0.9	0.8	64.3	173.0	-148.0	-110.0

Table S4 *(continued)*. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **1PP mono-solvated** with **DMSO-d_6** calculated within the **IEFPCM of DMSO**.

Conf.	**ΔE[a] [kcal/mol]**	**ΔG[a] [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**	**α** (C_{Ar}-C*-O-H)	**β** (C_{Ar}-C*-CH_2-CH_3)	**δ_1** (C*-O··O=S)	**δ_2** (O··O=S-CH_3)
1PP-c7	1.22	2.01	0.9	0.4	95.0	173.2	96.7	-140.0
	1.31	1.83	0.8	0.6	73.0	173.2	-172.3	55.4
	1.33	1.50	0.8	1.0	80.7	173.0	166.0	50.0
1PP-c8	1.43	2.04	0.6	0.4	95.5	62.8	113.8	-136.2
	1.49	2.32	0.6	0.2	95.6	62.8	104.2	-139.6
	1.50	1.84	0.6	0.5	63.0	62.5	-148.1	-123.3
	1.52	2.23	0.5	0.3	62.1	62.5	-144.5	-114.0
	1.63	2.40	0.5	0.2	75.3	62.6	-176.8	59.2
	1.66	2.31	0.4	0.3	86.7	62.5	144.6	48.1
1PP-c9	2.79	3.21	0.1	0.1	69.9	-61.6	172.7	-132.9
	2.81	3.22	0.1	0.1	58.2	-61.8	-165.1	-117.1
	2.99	3.95	0.0	0.0	63.7	-61.7	-176.4	49.0
	3.13	3.79	0.0	0.0	62.0	-62.2	-27.3	-114.9

[a] referenced to E = -978.602424 hartree and G = -978.653422 hartree

Table S5. Comparison of populations for different sets of conformers of **1PP** in DMSO. The full set summarizes the populations for each conformer over all solvent orientations from Table S4. The random selection of conformers refers to those conformers highlighted in red in Table S4.

	PCM (Tab. S3)		**Full Set (Tab. S4)**		**Lowest Energy Conformer**		**Random**	
	pop-ΔE [%]	**pop-ΔG [%]**	**pop-ΔE [%]**	**pop-ΔG [%]**	**pop-ΔE [%]**	**pop-ΔG [%]**	**pop-ΔE [%]**	**pop-ΔG [%]**
c1	35.6	35.1	39.5	50.1	31.0	45.9	40.5	52.4
c2	23.8	19.9	23.8	14.4	16.9	9.5	20.3	12.5
c3	4.5	3.3	6.4	4.8	4.7	3.1	4.8	5.5
c4	11.5	13.8	8.5	7.9	29.5	20.9	11.5	12.8
c5	9.4	8.5	10.1	11.8	7.0	6.9	10.1	10.6
c6	2.4	1.8	2.9	4.3	3.1	6.9	3.4	2.3
c7	6.0	6.5	5.4	4.7	4.7	5.2	5.8	2.3
c8	5.7	10.1	3.2	1.9	2.8	1.5	3.4	1.5
c9	1.1	0.9	0.2	0.1	0.3	0.1	0.3	0.1

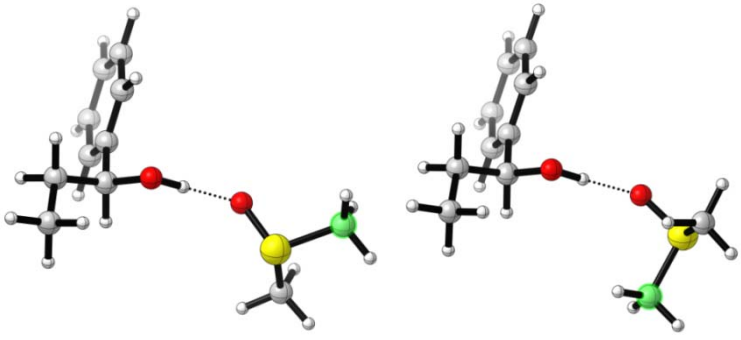


Figure S2. Structures of mono-solvated **1PP-c1··DMSO** with $\delta_2 < 0$ (left) and $\delta_2 > 0$ (right). The methyl group highlighted in green is used for the angle definition.

Table S6. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **1PP mono-solvated** with **ACN-d_3** calculated within the **IEFPCM of acetonitrile**.

Conf.	**α** (C_{Ar}-C*-O-H)	**β** (C_{Ar}-C*-CH_2-CH_3)	**ΔE_{ZPC}[a] [kcal/mol]**	**ΔG_{298K}[a] [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**
1PP-c1··ACN	-66.7	173.2	0.00	0.00	42.1	85.1
1PP-c2··ACN	-62.0	63.4	0.37	1.62	22.5	5.5
1PP-c3··ACN	-68.3	-64.0	1.24	2.56	5.2	1.1
1PP-c4··ACN	-148.2	174.9	0.88	2.05	9.6	2.7
1PP-c5··ACN	-174.1	64.5	0.95	2.37	8.5	1.5
1PP-c6··ACN	-172.2	-62.4	1.55	2.73	3.1	0.8
1PP-c7··ACN	78.2	173.3	1.22	2.16	5.4	2.2
1PP-c8··ACN	75.8	62.7	1.53	2.65	3.2	1.0
1PP-c9··ACN	69.8	-62.3	2.72	4.32	0.4	0.1

[a] referenced to E = -558.128363 hartree and G= -558.175844 hartree

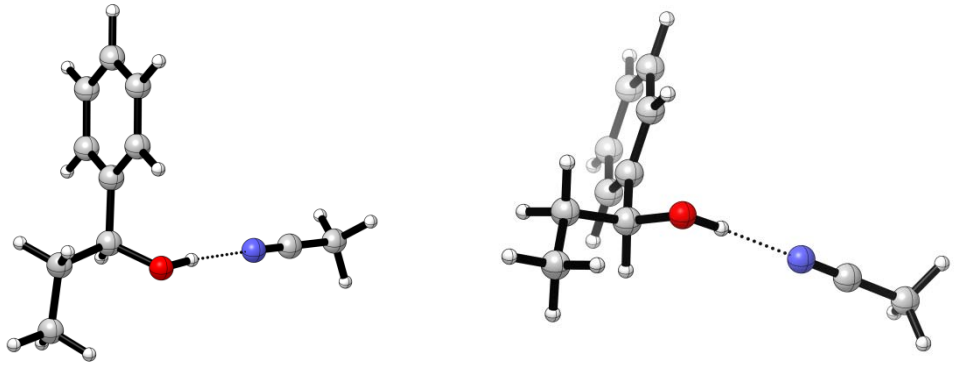


Figure S3. Structure of conformer **1PP-c1··ACN** in two different views.

1.3 Dimerization of 1PP

Table S7. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **dimers of 1PP** calculated within the **IEFPCM of chloroform**. Dimers with c9 as donor were not built due to energies being expected to be very high.

don	acc	α_{donor} (C_{Ar}-C*-O-H)	β_{donor} (C_{Ar}-C*-CH_2-CH_3)	$\alpha_{acceptor}$ (C_{Ar}-C*-O-H)	$\beta_{acceptor}$ (C_{Ar}-C*-CH_2-CH_3)	ΔE_{ZPC}[a] [kcal/mol]	ΔG_{298K}[a] [kcal/mol]	pop-ΔE [%]	pop-ΔG [%]
c1	c1	-61.2	173.9	-58.6	174.0	0.03	0.00	15.6	23.0
c1	c2	-63.8	173.9	-49.1	64.9	0.00	0.12	16.3	18.7
c1	c3	-62.6	174.1	-53.9	-62.2	1.03	1.27	2.9	2.7
c1	c4	-65.7	173.8	178.5	176.4	0.71	1.20	4.9	3.0
c1	c5	-63.3	173.7	174.2	64.9	0.97	1.69	3.2	1.3
c1	c6	-62.1	173.9	176.1	-61.0	1.69	1.94	0.9	0.9
c1	c7	-62.8	173.8	52.2	173.5	0.93	0.83	3.4	5.7
c1	c8	-64.4	174.1	55.8	63.4	1.10	1.41	2.5	2.1
c1	c9	-66.5	173.2	79.3	-63.1	2.04	2.73	0.5	0.2
c2	c1	-55.6	63.9	-58.9	174.1	0.44	1.01	7.8	4.2
c2	c2	-58.1	63.6	-50.0	64.8	0.40	1.21	8.2	3.0
c2	c3	-58.0	63.7	-55.6	-62.2	1.36	1.33	1.6	2.4
c2	c4	-60.2	63.5	178.4	176.3	1.15	1.27	2.3	2.7
c2	c5	-60.3	63.6	175.1	65.1	1.31	1.82	1.8	1.1
c2	c6	-59.9	63.5	175.0	-61.1	2.03	2.89	0.5	0.2
c2	c7	-63.1	63.3	55.1	173.9	1.43	1.13	1.5	3.4
c2	c8	-62.9	63.1	63.9	62.9	1.44	1.63	1.4	1.5
c2	c9	-60.3	63.5	73.9	-63.6	2.48	2.63	0.2	0.3
c3	c1	-62.6	-63.9	-58.8	173.9	1.20	1.01	2.1	4.2
c3	c2	-65.0	-64.0	-49.3	65.0	1.16	1.40	2.3	2.1
c3	c3	-62.8	-63.7	-54.6	-62.2	2.20	2.42	0.4	0.4
c3	c4	-62.8	-63.9	177.3	176.2	1.91	1.83	0.6	1.0
c3	c5	-69.1	-64.5	173.8	65.0	2.05	2.16	0.5	0.6
c3	c6	-59.9	-63.4	175.9	-61.2	2.81	3.40	0.1	0.1
c3	c7	-65.9	-64.0	53.9	173.3	2.05	2.00	0.5	0.8
c3	c8	-69.6	-64.2	64.7	63.0	2.25	2.82	0.4	0.2
c3	c9	-65.8	-64.2	74.8	-63.4	3.26	3.50	0.1	0.1
c4	c1	-155.7	174.3	-40.2	175.4	1.81	2.56	0.8	0.3
c4	c2	-153.7	175.1	-46.6	65.2	1.29	1.42	1.8	2.1
c4	c3	-153.1	174.9	-52.0	-61.8	2.40	2.59	0.3	0.3
c4	c4	170.9	176.0	-145.0	175.3	1.78	2.16	0.8	0.6
c4	c5	171.9	176.1	-175.8	64.6	1.85	2.15	0.7	0.6
c4	c6	-139.9	174.9	169.1	-60.8	2.78	2.87	0.1	0.2
c4	c7	168.6	175.8	70.2	172.3	2.36	3.28	0.3	0.1
c4	c8	170.3	176.0	69.6	62.5	2.47	3.01	0.2	0.1
c4	c9	not obtained							
c5	c1	-175.6	64.8	-57.3	171.7	1.61	1.32	1.1	2.5
c5	c2	-177.2	64.6	-52.5	64.7	1.37	1.93	1.6	0.9
c5	c3	-174.7	64.4	-54.0	-62.0	2.58	2.87	0.2	0.2
c5	c4	171.9	176.1	-175.8	64.6	1.85	2.16	0.7	0.6

Table S7 *(continued)*. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **dimers of 1PP** calculated within the **IEFPCM of chloroform**. Dimers with c9 as donor were not built due to energies being expected to be very high.

don	acc	α_{donor} (C_{Ar}-C*-O-H)	β_{donor} (C_{Ar}-C*-CH_2-CH_3)	$\alpha_{acceptor}$ (C_{Ar}-C*-O-H)	$\beta_{acceptor}$ (C_{Ar}-C*-CH_2-CH_3)	ΔE_{ZPC}[a] [kcal/mol]	ΔG_{298K}[a] [kcal/mol]	pop-ΔE [%]	pop-ΔG [%]
c5	c5	-173.1	64.6	170.1	65.0	1.91	2.03	0.6	0.7
c5	c6	-175.0	64.5	170.0	-61.1	2.83	3.00	0.1	0.1
c5	c7	-176.4	64.4	67.1	173.7	2.25	2.54	0.4	0.3
c5	c8	-176.0	64.5	63.7	63.1	2.21	2.32	0.4	0.5
c5	c9	-176.6	64.4	76.1	-63.3	3.46	3.99	0.0	0.0
c6	c1	-169.5	-62.1	-60.1	171.9	2.00	2.16	0.6	0.6
c6	c2	-171.4	-62.3	-52.4	64.9	1.80	2.13	0.8	0.6
c6	c3	-170.8	-62.6	-53.1	-61.7	3.00	3.48	0.1	0.1
c6	c4	-169.4	-62.6	-167.3	175.9	3.36	4.66	0.1	0.0
c6	c5	-169.5	-62.0	170.6	64.7	2.35	2.90	0.3	0.2
c6	c6	-167.3	-62.1	171.2	-61.0	3.59	4.06	0.0	0.0
c6	c7	-168.7	-62.4	52.6	173.4	2.74	2.85	0.2	0.2
c6	c8	-170.8	-62.3	66.2	63.2	2.62	3.00	0.2	0.1
c6	c9	-170.9	-62.4	76.4	-63.2	3.82	4.44	0.0	0.0
c7	c1	62.2	172.8	-55.2	173.7	1.78	2.58	0.8	0.3
c7	c2	66.2	172.5	-51.3	64.9	1.86	2.46	0.7	0.4
c7	c3	75.0	173.7	-51.7	-61.1	2.78	3.27	0.1	0.1
c7	c4	80.2	172.1	170.6	175.9	2.84	3.82	0.1	0.0
c7	c5	69.3	172.2	167.4	64.8	2.44	3.29	0.3	0.1
c7	c6	80.4	172.6	171.3	-60.7	3.76	4.93	0.0	0.0
c7	c7	73.0	173.4	70.9	173.0	2.64	3.40	0.2	0.1
c7	c8	70.7	173.3	67.6	62.9	2.65	3.24	0.2	0.1
c7	c9	73.5	172.9	73.5	-63.2	3.85	4.51	0.0	0.0
c8	c1	62.7	62.7	-55.2	173.8	1.84	2.26	0.7	0.5
c8	c2	68.8	62.6	-51.7	64.7	2.00	2.96	0.6	0.2
c8	c3	69.8	62.4	-52.8	-59.3	3.33	4.17	0.1	0.0
c8	c4	75.7	63.1	170.5	175.9	3.20	3.81	0.1	0.0
c8	c5	69.8	62.5	167.0	64.8	2.63	3.35	0.2	0.1
c8	c6	73.0	62.6	176.8	-61.4	4.30	6.46	0.0	0.0
c8	c7	75.7	62.6	53.0	173.9	2.80	3.33	0.1	0.1
c8	c8	52.2	63.5	74.7	62.5	2.91	3.70	0.1	0.0
c8	c9	71.3	62.3	80.7	-63.0	3.68	4.30	0.0	0.0

[a] referenced to E = -850.714945 hartree (dimer c1-c2) and G= -850.772293 hartree (dimer c1-c1)

2. Additional spectra of 1PP

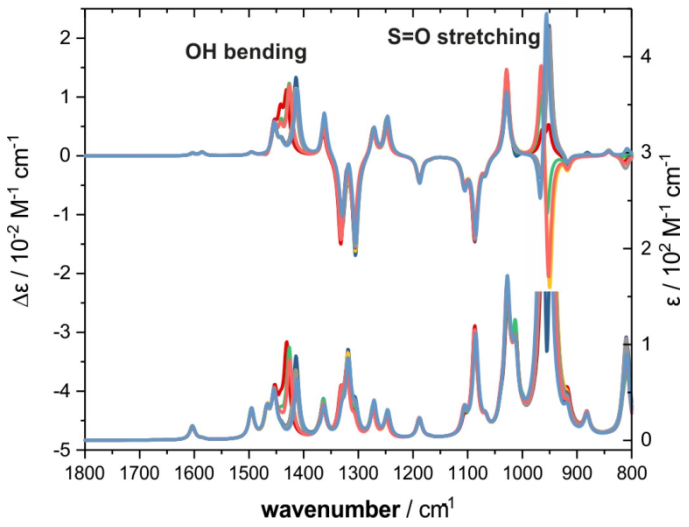


Figure S4. Comparison for the effect of different solvent orientations on the single-conformer IR and VCD spectra of **1PP-c1··DMSO-d$_6$**.

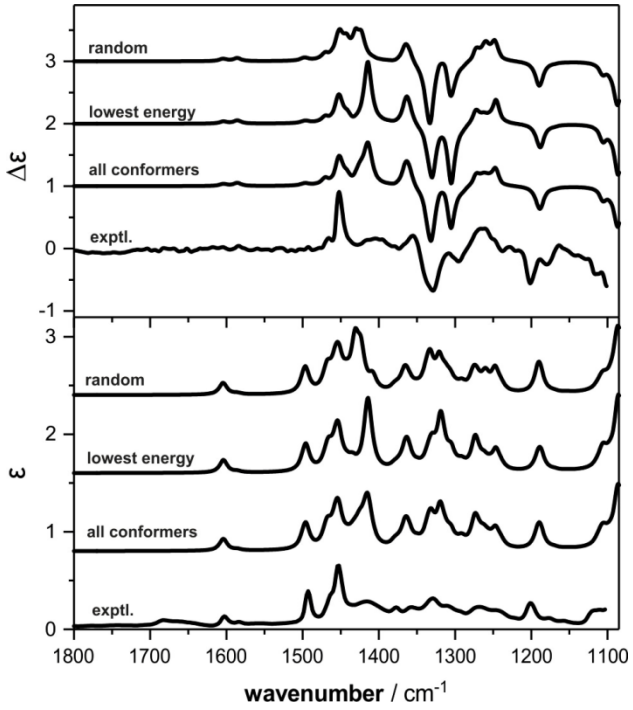


Figure S5. Comparison for the effect of different Boltzmann weighting schemes (cf. Table S5) on the prediction of the IR and VCD spectra of **1PP··DMSO-d$_6$**. Molar ellipticity ε in 10^2 M^{-1} cm^{-1} and differential molar ellipticity Δε in 10^{-2} M^{-1} cm^{-1}.

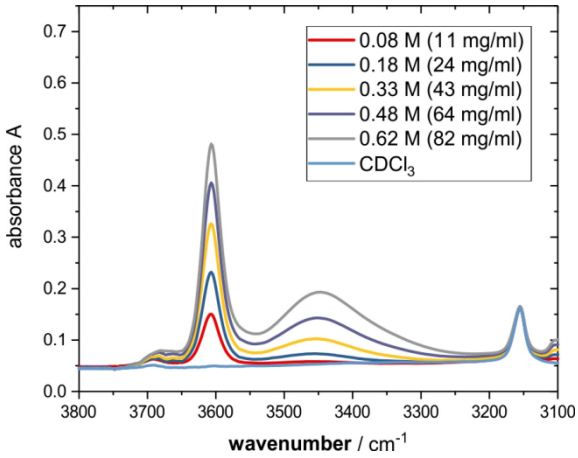


Figure S6. Exemplifying the concentration dependence of the IR spectra of **1PP-c1** in the OH-stretching range. Spectra are not background corrected.

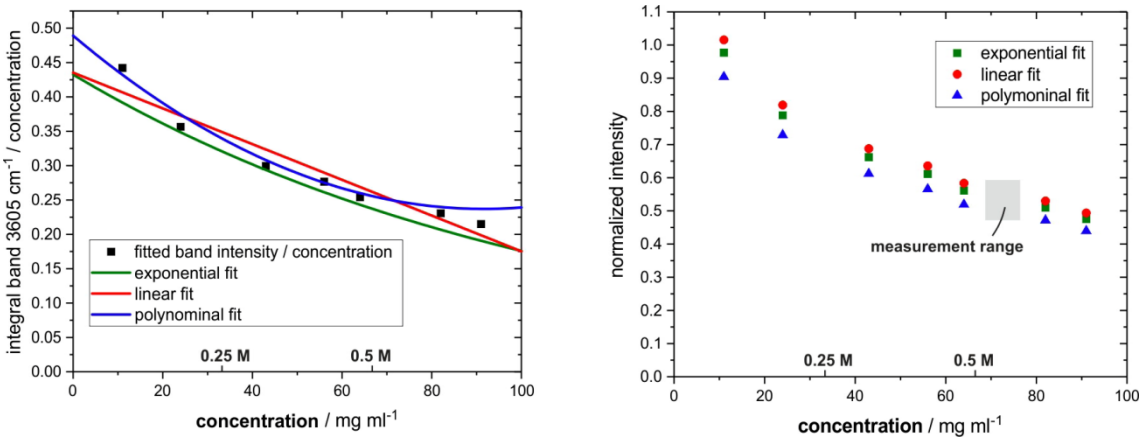


Figure S7. Fitted band intensities of the monomer OH-stretching mode at~3605 cm^{-1} and possible fits of the data points (left); resulting relative intensities after normalization.

4. Vibrational energy distribution

Table S8. Vibrational energy distribution of **monomeric 1PP** (IEFPCM of ACN). Only contributions >10% shown. σ: stretching, δ: bending, τ: torsional. Atom numbering see Figure S8. For color code see main text.

ν	ν_{scaled}	D	R	Contributions				
1637.4	1604.6	9.1	0.6	σ(C_5-C_4) 30				
1618.8	1586.4	1.2	0.9	σ(C_1-C_6) -27	σ(C_2-C_3) 20			
1527.1	1496.6	29.9	1.3	δ(H_7-C_1-C_2) -19	δ(H_8-C_2-C_3) -16	δ(H_9-C_4-C_5) 16	δ(H_{10}-C_5-C_6) 20	
1497.6	1467.7	33.5	-3.2	δ(H_{16}-C_{14}-H_{15}) -12	δ(H_{18}-C_{17}-H_{20}) -18	δ(H_{20}-C_{17}-H_{19}) 48		
1486.7	1457.0	0.9	-4.4	δ(H_{11}-C_4-C_1) 12	δ(H_{18}-C_{17}-H_{20}) 17	δ(H_{19}-C_{17}-H_{18}) -24		
1484.8	1455.1	57.0	20.7	δ(H_{11}-C_4-C_1) 12	δ(H_{18}-C_{17}-H_{20}) -18	δ(H_{19}-C_{17}-H_{18}) 26		
1470.1	1440.7	5.5	0.2	δ(H_{16}-C_{14}-H_{15}) 70				
1407.2	**1379.1**	**36.8**	**40.3**	σ(C_{14}-C_{12}) -10	**δ(H_{22}-O_{21}-C_{12}) 14**	**δ(H_{13}-C_{12}- O_{21}) -14**	τ(C_{12}-C_3-C_{14}-H_{13}) -14	
1401.8	1373.8	12.7	9.4	δ(H_{18}-C_{17}-H_{20}) 20	δ(H_{19}-C_{17}-H_{18}) 18	δ(H_{20}-C_{17}-H_{19}) 12		
1391.3	**1363.5**	**15.2**	**-10.1**	**δ(H_{13}-C_{12}- O_{21})** 28	τ(C_{12}-C_3-C_{14}-H_{13}) 23			
1353.0	**1326.0**	**3.6**	**0.7**	δ(H_8-C_2-C_3) -20	δ(H_9-C_4-C_5) -19			
1338.8	**1312.1**	**14.5**	**8.6**	σ(C_5-C_4) 10	+ many small contributions			
1320.4	**1294.0**	**104.7**	**-50.9**	**δ(H_{22}-O_{21}-C_{12}) -16**	δ(H_{15}-C_{14}-C_{17}) 31	τ(H_{16}-C_{14}-C_{12}-C_3) -18		
1298.0	1272.0	65.2	11.5	σ(C_2-C_3) 15	σ(C_{12}-C_3) 10	δ(H_{13}-C_{12}- O_{21}) 10		
1254.3	**1229.2**	**107.6**	**9.4**	**δ(H_{22}-O_{21}-C_{12}) 18**	τ(C_{12}-C_3-C_{14}-H_{13}) 13			
1211.4	1187.2	10.6	-11.6	σ(C_2-C_3) -13	σ(C_{12}-C_3) 11			
1195.2	1171.3	0.6	-0.5	δ(H_7-C_1-C_2) 19	δ(H_8-C_2-C_3) -21	δ(H_9-C_4-C_5) 21	δ(H_{10}-C_5-C_6) -14	
1177.1	1153.5	0.5	0.0	σ(C_5-C_6) -10	δ(H_7-C_1-C_2) -16	δ(H_{10}-C_5-C_6) -19	δ(H_{11}-C_4-C_1) 39	
1120.8	**1098.4**	**30.3**	**-22.6**	**σ(O_{21}-C_{12}) -14**	τ(H_{19}-C_{17}-C_{14}-C_{12}) -15			
1103.6	1081.5	131.2	-50.5	σ(C_1-C_2) 10	τ(H_{20}-C_{17}-C_{14}-C_{12}) 12			
1082.5	**1060.8**	**25.3**	**2.3**	τ(H_{20}-C_{17}-C_{14}-C_{12}) -10				
1045.9	1025.0	32.0	-1.0	σ(C_1-C_6) 16	σ(C_5-C_6) 19	δ(H_{10}-C_5-C_6) 10	δ(C_2-C_1-C_6) -10	δ(C_6-C_5-C_4) -15
1041.3	1020.4	199.1	42.2	σ(C_{14}-C_{12}) -21	σ(C_{17}-C_{14}) 50			
1017.5	997.2	1.1	-0.1	σ(C_1-C_6) 13	σ(C_6-C_5) 16	δ(C_1-C_6-C_5) -17	δ(C_2-C_1-C_6) 12	δ(C_6-C_5-C_4) 24
1007.9	987.7	0.9	-0.1	τ(H_7-C_1-C_2-C_3) 17	τ(H_9-C_4-C_3-C_{12}) 10	τ(H_{10}-C_5-C_6-C_1) 19	τ(H_{11}-C_6-C_1-C_2) -26	τ(C_3-C_2-C_1-C_6) -13

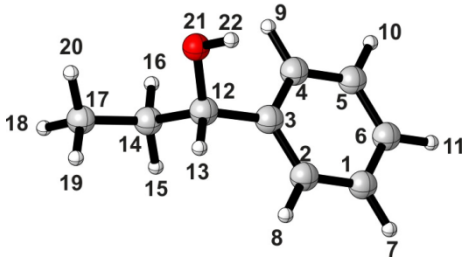


Figure S8. Atom numbering for vibrational energy distribution analysis.

Table S9. Vibrational energy distribution of **ACN-monosolvated 1PP** (IEFPCM of ACN), ACN modes removed from table. Only contributions >10% shown. σ: stretching, δ: bending, τ: torsional. Atom numbering see Figure S8. For color code see main text.

ν	ν_{scaled}	D	R	Contrib				
1636.7	1604.0	13.7	0.9	σ(C_5-C_4) 30				
1618.3	1585.9	1.2	1.5	σ(C_1-C_6) -26	σ(C_2-C_3) 19	δ(C_1-C_2-C_3) -11		
1526.5	1496.0	33.3	1.4	δ(H_7-C_1-C_2) -18	δ(H_8-C_2-C_3) -16	δ(H_9-C_4-C_5) 15	δ(H_{10}-C_5-C_6) 19	
1497.4	1467.5	32.1	-1.4	δ(H_{16}-C_{14}-H_{15}) -13	δ(H_{18}-C_{17}-H_{20}) -16	δ(H_{20}-C_{17}-H_{19}) 46	τ(H_{20}-C_{17}-C_{14}-C_{12}) 11	
1485.4	1455.7	2.5	0.9	δ(H_{11}-C_6-C_1) -18	δ(H_{18}-C_{17}-H_{20}) -10	δ(H_{19}-C_{17}-H_{18}) 16		
1483.7	1454.0	52.7	15.3	δ(H_{18}-C_{17}-H_{20}) -20	δ(H_{19}-C_{17}-H_{18}) 32	τ(H_{18}-C_{17}-C_{14}-C_{12}) -11		
1470.8	1441.4	5.4	2.7	δ(H_{16}-C_{14}-H_{15}) 68				
1430.1	**1401.5**	**62.6**	**36.0**	**δ(H_{22}-O_{21}-C_{12}) 43**	τ(C_2-C_3-C_{12}-H_{13}) 32			
1399.4	1371.4	3.7	-1.2	δ(H_{18}-C_{17}-H_{20}) 36	δ(H_{19}-C_{17}-H_{18}) 28	δ(H_{20}-C_{17}-H_{19}) 27		
1392.2	**1364.4**	**38.4**	**16.6**	δ(H_{13}-C_{12}-C_3) 48				
1355.8	**1328.7**	**14.4**	**-22.9**	δ(H_8-C_2-C_3) -18	δ(H_9-C_4-C_5) -16	**τ(H_{16}-C_{14}-C_{12}-O_{21})** 19		
1343.6	1316.7	101.6	5.4	σ(C_5-C_4) 10	**δ(H_{22}-O_{21}-C_{12})** -10	**τ(H_{16}-C_{14}-C_{12}-O_{21})** -12		
1331.5	**1304.9**	**48.6**	**-59.6**	δ(H_{15}-C_{14}-C_{17}) 34	τ(C_2-C_3-C_{12}-H_{13}) 17	**τ(H_{15}-C_{14}-C_{12}-O_{21}) -11**		
1298.3	1272.4	48.8	15.1	σ(C_2-C_3) 16	δ(H_{13}-C_{12}- C_3) -12			
1269.3	**1243.9**	**46.3**	**21.7**	δ(H_{15}-C_{14}-C_{17}) -13	τ(C_2-C_3-C_{12}-H_{13}) 20	**τ(H_{16}-C_{14}-C_{12}-O_{21}) 14**		
1212.7	1188.4	25.3	-15.6	σ(C_2-C_3) -10	σ(C_{12}-C_3) 35			
1194.4	1170.5	0.9	-0.7	δ(H_7-C_1-C_2) 19	δ(H_8-C_2-C_3) -20	δ(H_9-C_4-C_5) 21	δ(H_{10}-C_5-C_6) -14	
1176.1	1152.6	0.6	0.1	σ(C_5-C_6) -10	δ(H_7-C_1-C_2) -17	δ(H_{10}-C_5-C_6) -20	δ(H_{11}-C_6-C_1) 37	
1126.2	**1103.7**	**34.6**	**-18.6**	**σ(O_{21}-C_{12}) -16**	τ(H_{19}-C_{17}-C_{14}-C_{12}) **-15**	τ(C_{17}-C_{14}-C_{12}-C_{21}) **10**		
1106.5	1084.4	163.9	-53.7	σ(C_{14}-C_{12}) 17	τ(H_{20}-C_{17}-C_{14}-C_{12}) 17			
1088.7	**1066.9**	**19.1**	**-6.2**	σ(C_2-C_1) **15**	σ(C_5-C_4) **-11**			
1047.4	1026.5	191.0	50.2	σ(C_{14}-C_{12}) -19	σ(C_{17}-C_{14}) 48	σ(O_{21}-C_{12}) 13		
1045.9	1024.9	38.6	-0.9	σ(C_1-C_6) 15	σ(C_5-C_6) 18	δ(C_4-C_5-C_6) -16	δ(H_{10}-C_5-C_6) 10	δ(C_2-C_1-C_6) -10
1017.2	996.9	0.7	-0.2	σ(C_1-C_6) -12	σ(C_5-C_6) -15	δ(C_4-C_5-C_6) -24	δ(C_1-C_6-C_5)18	δ(C_2-C_1-C_6) -12
1006.3	986.2	0.9	0.0	τ(H_7-C_1-C_6-C_5) 16	τ(H_{10}-C_5-C_6-C_1) -25	τ(H_{11}-C_6-C_5-C_4) -27	τ(C_4-C_5-C_6-C_1) 15	

5. Spectra of 1PE, 1P2P and 2P1P

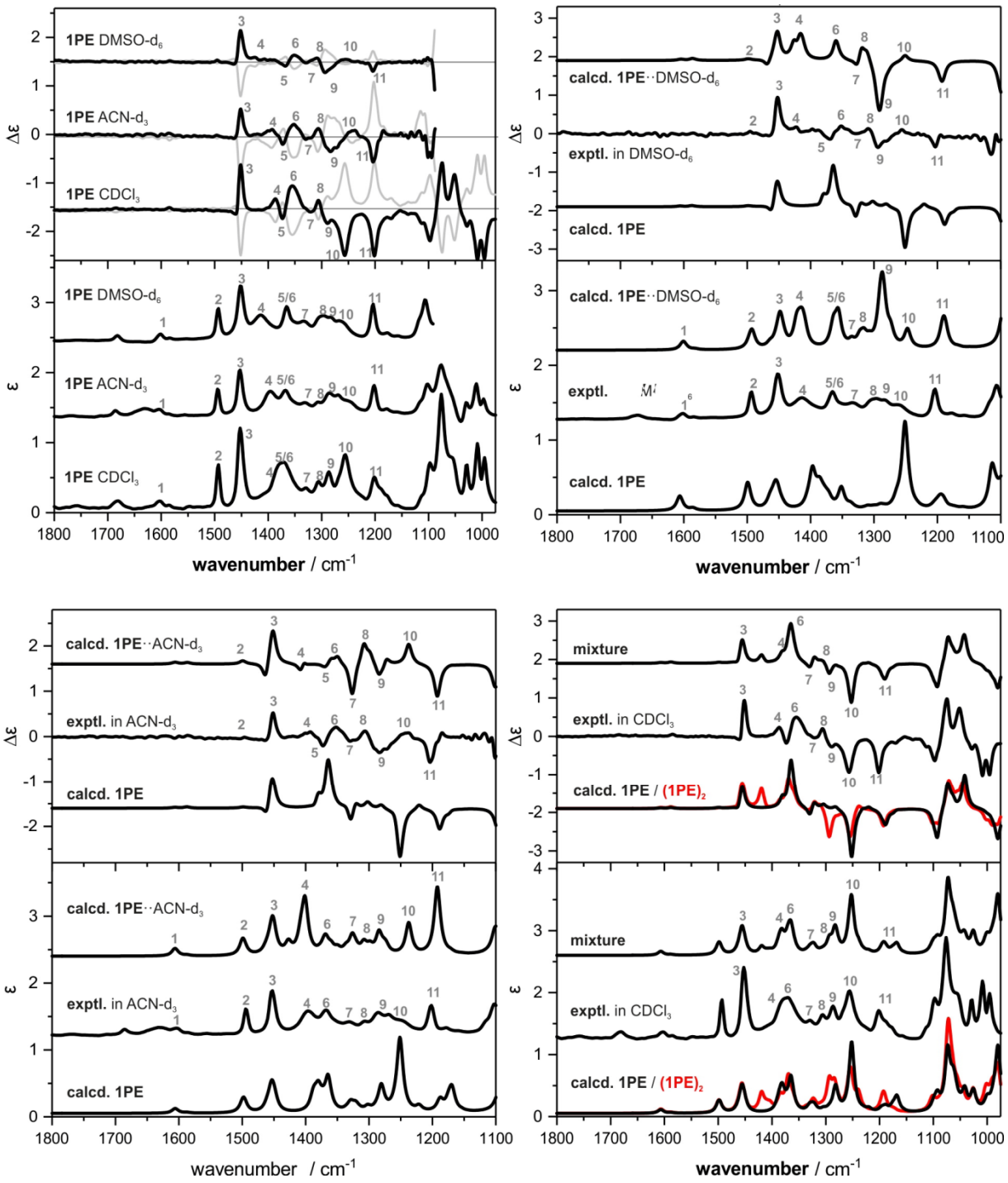


Figure S9. Comparison of the experimental and computed spectra of **1PE**. Experimental recorded in $CDCl_3$ (0.54 M), ACN-d_3 (0.71 M) and DMSO-d_6 (1.19 M) with 100 µm path length (black = (S)-**1PE**; grey = (R)-**1PE**).. Computations carried out considering only implicit solvation with IEFPCM of the respective solvent or by explicit treatment of intermolecular interactions (solvation/dimerization). Molar ellipticity ε in 10^2 M^{-1} cm^{-1} and differential molar ellipticity Δε in 10^{-2} M^{-1} cm^{-1}.

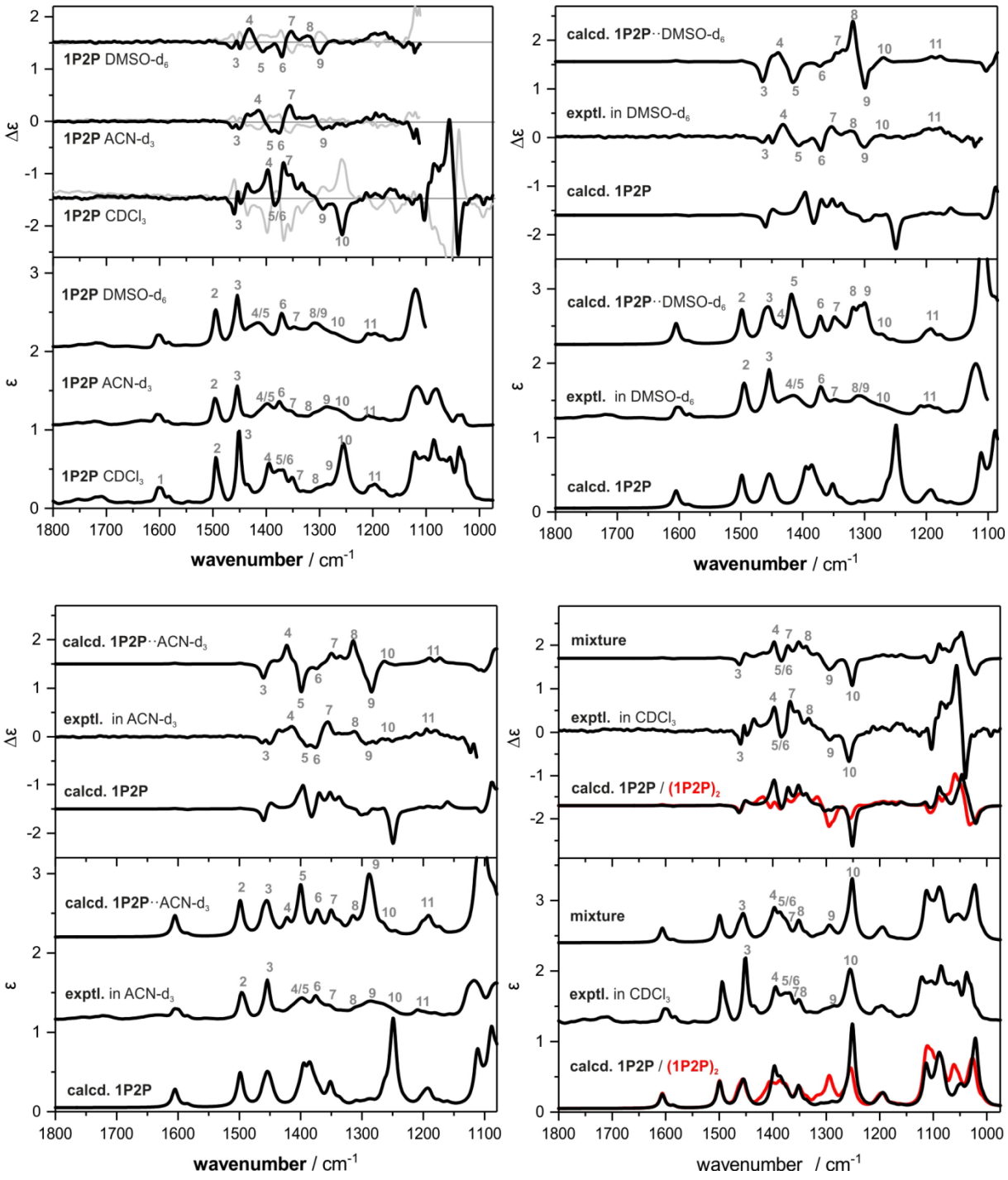


Figure S10. Comparison of the experimental and computed spectra of **1P2P**. Experimental recorded in $CDCl_3$ (0.62 M), ACN-d_3 (1.32 M) and DMSO-d_6 (0.92 M) with 100 µm path length (black = (S)-**1P2P**; grey = (R)-**1P2P**). Computations carried out considering only implicit solvation with IEFPCM of the respective solvent or by explicit treatment of intermolecular interactions (solvation/dimer). Molar ellipticity ε in 10^2 M^{-1} cm^{-1} and differential molar ellipticity Δε in 10^{-2} M^{-1} cm^{-1}.

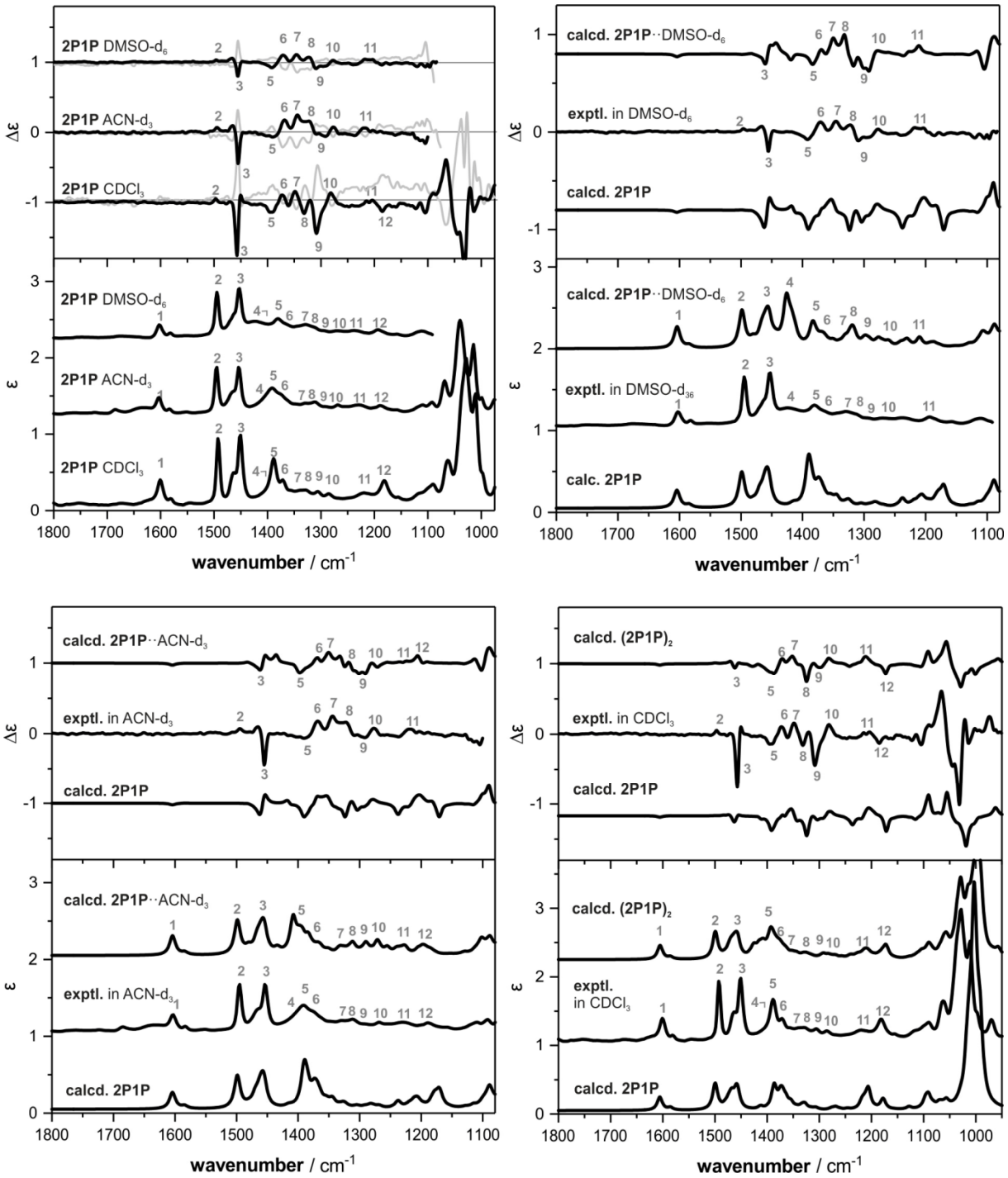


Figure S11. Comparison of the experimental and computed spectra of **2P1P**. Experimental recorded in $CDCl_3$ (0.56 M), ACN-d_3 (0.84 M) and DMSO-d_6 (1.22 M) with 100 µm path length (black = (S)-**2P1P**; grey = (R)-**2P1P**). Computations carried out considering only implicit solvation with IEFPCM of the respective solvent or by explicit treatment of intermolecular interactions (solvation/dimerization). Molar ellipticity ε in 10^2 M^{-1} cm^{-1} and differential molar ellipticity Δε in 10^{-2} M^{-1} cm^{-1}.

6. Selected computational data on 1PE, 1P2P and 2P1P

6.1 1-Phenyl ethanol (1PE)

Table S10. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated 1PE** calculated within the **IEFPCM of chloroform**.

Conf.	**α** (C_{Ar}-C*-O-H)	**ΔE_{ZPC}[a] [kcal/mol]**	**ΔG_{298K}[a] [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**
1PE-c1	-55.8	0.00	0.00	73.5	67.3
1PE-c2	173.7	0.81	0.55	18.9	26.5
1PE-c3	59.7	1.35	1.41	7.6	6.2

[a] referenced to E=-386.058666hartree and G=-386.09215hartree

Table S11. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated 1PE** calculated within the **IEFPCM of DMSO**.

Conf.	**α** (C_{Ar}-C*-O-H)	**ΔE_{ZPC}[a] [kcal/mol]**	**ΔG_{298K}[a] [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**
1PE-c1	-57.0	0.00	0.00	64.9	58.0
1PE-c2	174.8	0.56	0.33	25.3	33.3
1PE-c3	81.7	1.12	1.13	9.7	8.7

[a] referenced to E=-386.060548 hartree and G=-386.094029 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-monosolvated 1PE** calculated within the **IEFPCM of ACN**.

Conf.	**α** (C_{Ar}-C*-O-H)	**ΔE_{ZPC}[a] [kcal/mol]**	**ΔG_{298K}[a] [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**
1PE-c1··ACN	-64.1	5.40	6.16	18.8	30.5
1PE-c2··ACN	79.5	0.66	1.08	34.4	46.9
1PE-c3··ACN	-176.1	0.00	0.00	46.8	22.5

[a] referenced to E=-386.060471 hartree and G=-386.093949 hartree

Table S13. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the their Boltzmann populations of **DMSO-monosolvated 1PE** calculated within the **IEFPCM of DMSO**.

Conf.	**α** (C_{Ar}-C*-O-H)	**ΔE_{ZPC}[a] [kcal/mol]**	**ΔG_{298K}[a] [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**
1PE-c1··DMSO-1	-66.2	0.00	0.43	38.0	19.5
1PE-c1··DMSO-2	-65.6	0.18	0.00	28.0	40.5
1PE-c2··DMSO-1	-175.9	0.54	0.25	15.3	26.4
1PE-c2··DMSO-2	-175.3	0.74	0.85	10.9	9.7
1PE-c3··DMSO-1	76.45	1.34	1.71	3.9	2.3
1PE-c3··DMSO-2	76.9	1.36	1.91	3.8	1.6

[a] referenced to E=-939.306004 hartree and G=-939.354398 hartree

6.2 1-Phenyl-2-propanol (1P2P)

Table S14. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated 1P2P** calculated within the **IEFPCM of chloroform**.

Conf.	**α** (C_{Ar}-C*-O-H)	**β** (C_{Ar}-C*-CH_2-CH_3)	**ΔE_{ZPC}[a] [kcal/mol]**	**ΔG_{298K}[a] [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**
1P2P-c1	-56.1	-179.2	0.00	0.00	53.5	49.1
1P2P-c2	-175.7	-172.8	1.04	0.79	9.3	13.0
1P2P-c3	-58.8	-66.8	1.07	1.04	8.8	8.5
1P2P-c4	177.0	-67.1	1.08	0.98	8.7	9.4
1P2P-c5	68.7	-65.6	1.21	1.13	6.9	7.3
1P2P-c6	65.5	-174.5	1.30	1.14	6.0	7.2
1P2P-c7	65.7	64.2	1.52	1.73	4.1	2.7
1P2P-c8	176.1	55.9	2.12	2.09	1.5	1.5
1P2P-c9	-61.2	56.1	2.25	2.14	1.2	1.3

[a] referenced to E=-425.358257 hartree and G=-425.393671 hartree

6.3 2-Phenyl-1-propanol (2P1P)

Table S15. Geometries, relative zero-point-corrected electronic and Gibbs free energies (ΔE_{ZPC} and ΔG_{298K}) and the corresponding Boltzmann populations of **isolated 2P1P** calculated within the **IEFPCM of chloroform**.

Conf.	**α** (C_{Ar}-C*-O-H)	**β** (C_{Ar}-C*-CH_2-CH_3)	**ΔE_{ZPC}[a] [kcal/mol]**	**ΔG_{298K}[a] [kcal/mol]**	**pop-ΔE [%]**	**pop-ΔG [%]**
2P1P-c1	59.7	-60.8	0.00	0.00	39.9	36.1
2P1P-c2	67.8	-174.6	0.73	0.79	11.6	9.6
2P1P-c3	-179.9	-171.9	0.76	0.66	11.0	11.8
2P1P-c4	-72.3	-171.1	0.77	0.54	11.0	14.5
2P1P-c5	-64.7	64.3	0.90	1.10	8.7	5.6
2P1P-c6	-61.6	-58.5	1.01	0.92	7.2	7.6
2P1P-c7	175.3	-63.5	1.03	0.72	7.0	10.8
2P1P-c8	-175.2	69.8	1.77	1.58	2.0	2.5
2P1P-c9	74.4	68.5	1.89	1.90	1.6	1.5

[a] referenced to E=-425.351971 hartree and G=-425.387422 hartree

7. Cartesian coordinates of selected structures

1PP-c1 (pcm chloroform)

C	2.45234000	-1.17642000	0.18694400
C	1.08486500	-1.19592400	0.44867300
C	0.29700700	-0.06702900	0.22097700
C	0.90816900	1.09074300	-0.26711500
C	2.27471900	1.11513300	-0.52513000
C	3.05130400	-0.01942700	-0.30114600
H	3.04957500	-2.06176300	0.37144500
H	0.62528600	-2.09872300	0.83757500
H	0.30937400	1.97761700	-0.43651500
H	2.73527400	2.02121300	-0.90158100
H	4.11610200	0.00073600	-0.50096800
C	-1.19835400	-0.11386500	0.47537500
H	-1.40856200	-0.97536300	1.12262700
C	-2.00168700	-0.27636600	-0.81687100
H	-1.59749500	-1.13808300	-1.35543900
H	-1.81945200	0.60074600	-1.44598800
C	-3.50165700	-0.46184200	-0.58630200
H	-4.02492500	-0.59052000	-1.53654300
H	-3.69891800	-1.34739500	0.02463300
H	-3.93319900	0.40058600	-0.07675500
O	-1.67142400	1.08051300	1.11800400
H	-1.18189400	1.19681400	1.94104600

1PP-c1··DMSO (pcm DMSO)
Lowest energy structure

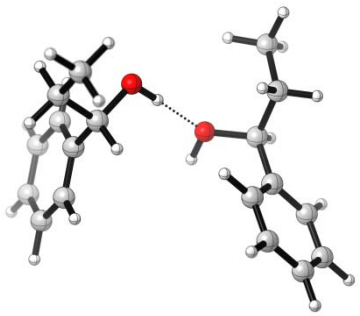
C	2.94328500	-1.97739600	-1.12937800
C	2.21901300	-0.79130300	-1.21964400
C	1.83267200	-0.09766500	-0.07148100
C	2.18157500	-0.62212000	1.17502800
C	2.90314700	-1.80847800	1.27019300
C	3.28851200	-2.49005200	0.11789200
H	3.23089200	-2.50388700	-2.03215100
H	1.94623800	-0.40275400	-2.19558000
H	1.87514600	-0.10112600	2.07394300
H	3.16399000	-2.20314700	2.24558600
H	3.84758700	-3.41537900	0.19210300
C	1.08023600	1.21947600	-0.18787800
H	0.59431400	1.24208000	-1.17310900
C	2.03289900	2.41724500	-0.10261500
H	2.84282300	2.25875600	-0.82035000
H	2.49104100	2.41839300	0.89225700
C	1.35434300	3.75973400	-0.37484900
H	2.07591500	4.57804800	-0.31587800
H	0.91031200	3.77907700	-1.37438500
H	0.56151500	3.95565200	0.34839000
O	0.09276900	1.37244700	0.82954500
H	-0.61671400	0.70955100	0.68638100
S	-3.26769700	0.02293700	-0.10950600
O	-1.94551300	-0.47390900	0.47955700
C	-3.65176000	-1.10074700	-1.48359300
H	-4.64500200	-0.85922200	-1.86144500
H	-2.90482600	-0.92135500	-2.25458800
H	-3.60236600	-2.12914100	-1.12759900
C	-4.56086100	-0.52638200	1.04114600
H	-4.42024300	0.03499300	1.96283600
H	-5.53277100	-0.29399000	0.60639400
H	-4.45112600	-1.59572000	1.21753800

1PP-c1··ACN (pcm ACN)

C	-1.67756100	-2.35646800	1.16917900
C	-1.29364700	-1.02034500	1.25354100
C	-1.07124500	-0.26457700	0.10139500
C	-1.23337000	-0.87810600	-1.14290700
C	-1.61403100	-2.21369800	-1.23180200
C	-1.83953600	-2.95770700	-0.07562700
H	-1.84254600	-2.92850200	2.07492500
H	-1.16127900	-0.56085100	2.22770400
H	-1.05035300	-0.30647900	-2.04468700
H	-1.73381000	-2.67567300	-2.20511000
H	-2.13350600	-3.99838900	-0.14504700
C	-0.69739100	1.20524300	0.20972600
H	-0.28815400	1.37674700	1.21427400
C	-1.91970600	2.11177200	0.03274200
H	-2.70140400	1.76097100	0.71238800
H	-2.30277300	1.97366500	-0.98390400
C	-1.63033500	3.58984100	0.29417900
H	-2.53550700	4.18912800	0.17107800
H	-1.26547200	3.74362300	1.31383200
H	-0.87564300	3.97324200	-0.39383900
O	0.27346200	1.59069800	-0.76628000
H	1.11166300	1.13663500	-0.57090200
C	3.94747300	-0.06568600	-0.00028300
N	2.89859500	0.35773600	-0.20463500
C	5.27407300	-0.60086600	0.25923300
H	5.63639900	-1.13291400	-0.62082300
H	5.96095000	0.21292800	0.49344100
H	5.23523100	-1.29028100	1.10309600

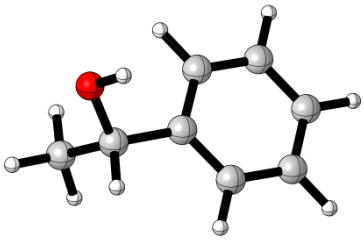
Dimer 1PP-c1··1PP-c1 (pcm chloroform)

C	-3.06091500	-2.79409000	-0.16855700
C	-2.54982800	-1.72893300	0.56842700
C	-2.61482300	-0.42291000	0.08039200
C	-3.19620600	-0.20443500	-1.17066100
C	-3.70531300	-1.26641700	-1.91154400
C	-3.64156500	-2.56523600	-1.41234100
H	-2.99920500	-3.80188100	0.22569000
H	-2.09115500	-1.91608700	1.53406700
H	-3.23871700	0.80296000	-1.56638200
H	-4.15232800	-1.08037900	-2.88142800
H	-4.03649600	-3.39219200	-1.99068400
C	-2.09242200	0.73519100	0.91582900
H	-1.38233100	0.32707500	1.64898200
C	-3.22082300	1.43025300	1.68453800
H	-3.78060600	0.66494900	2.22978900
H	-3.91178100	1.86479200	0.95475700
C	-2.72900700	2.50588600	2.65304500
H	-3.56797800	2.96162600	3.18425900
H	-2.05283100	2.08186800	3.40124500
H	-2.19291600	3.29575100	2.12559000
O	-1.43756800	1.72476000	0.12244900
H	-0.67292300	1.31426300	-0.31939400
C	4.68013200	-1.77523500	0.32919400
C	4.01033200	-0.98344100	-0.60034700
C	2.89183100	-0.23700300	-0.22916700
C	2.44803400	-0.30435100	1.09428700
C	3.11159000	-1.09740100	2.02364400
C	4.23177300	-1.83409400	1.64437900
H	5.54664000	-2.34970500	0.02339800
H	4.36053000	-0.94746700	-1.62660200
H	1.57536000	0.26255400	1.39589600
H	2.75563800	-1.14066600	3.04640200
H	4.74792200	-2.45232500	2.36923100
C	2.19439200	0.64678600	-1.24450500
H	2.56221400	0.38282700	-2.24287900
C	2.45349100	2.13519800	-1.01008600
H	3.53593900	2.27335500	-0.94020400
H	2.04035400	2.41026900	-0.03458300
C	1.88252000	3.03852100	-2.10370100
H	2.11859700	4.08500700	-1.89901600
H	2.30409300	2.78667500	-3.08089000
H	0.79790200	2.94622900	-2.17160600
O	0.76299700	0.45333500	-1.22610100
H	0.57150100	-0.47398500	-1.41338700



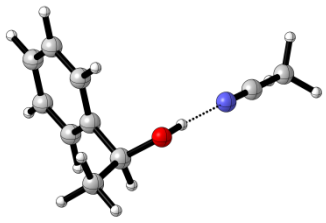
1PE-c1 (pcm chloroform)

C	-2.09591100	1.07847200	0.14941900
C	-0.71783300	1.24704500	0.25916300
C	0.14875300	0.16409800	0.11001400
C	-0.39210700	-1.09936900	-0.14237500
C	-1.76794600	-1.27224500	-0.24702800
C	-2.62470000	-0.18288300	-0.10417500
H	-2.75479300	1.93057600	0.26905100
H	-0.31195300	2.23199400	0.46542000
H	0.26959900	-1.95072900	-0.24897400
H	-2.17341600	-2.25854600	-0.44083100
H	-3.69668200	-0.31848400	-0.18530500
O	2.28971500	-0.65403900	0.98012100
H	1.87551600	-0.67297100	1.85147600
C	1.65077500	0.36782800	0.19666100
H	1.83518700	1.34268000	0.66364500
C	2.32529500	0.34726800	-1.16965000
H	2.16788600	-0.61648400	-1.65848300
H	1.91411200	1.13033300	-1.80878500
H	3.39887800	0.51266400	-1.06035700



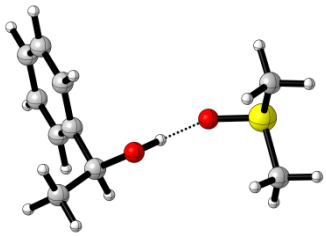
1PE-c1··ACN (pcm ACN)

C	1.99098800	-1.84611200	-1.08197600
C	1.45241400	-0.57381200	-1.26069400
C	1.18916900	0.25226800	-0.16755300
C	1.46995900	-0.22451200	1.11532000
C	2.00400300	-1.49594600	1.29862500
C	2.26858000	-2.31115400	0.19977400
H	2.18628200	-2.47494300	-1.94289300
H	1.23026100	-0.22108600	-2.26257500
H	1.25929000	0.40160900	1.97407100
H	2.21381800	-1.85257200	2.30053100
H	2.68279300	-3.30217800	0.34306000
O	-0.38493700	1.98426600	0.56522400
H	-1.14401300	1.39038800	0.42851400
C	0.63719000	1.65345100	-0.38019300
H	0.21974500	1.69929600	-1.39352400
C	1.72059600	2.72008200	-0.25585300
H	2.14956500	2.71144600	0.74892100
H	2.52202000	2.53927900	-0.97425700
H	1.29774700	3.70862700	-0.44659500
N	-2.79614900	0.31887800	0.18066300
C	-3.76241500	-0.28563600	0.03202000
C	-4.98416600	-1.05055100	-0.15715200
H	-4.85228500	-1.76020400	-0.97441400
H	-5.22279300	-1.59688800	0.75579700
H	-5.80780500	-0.37751700	-0.39697300



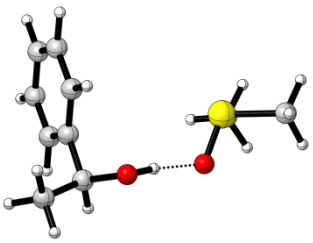
1PE-c1··DMSO (pcm DMSO)

C	3.46270000	-1.07477900	-1.20954500
C	2.56333900	-0.01150600	-1.24591600
C	1.89557400	0.40161500	-0.09249800
C	2.14070800	-0.27872300	1.10270600
C	3.03548900	-1.34339200	1.14309500
C	3.70195200	-1.74426400	-0.01321700
H	3.96977100	-1.38363600	-2.11636200
H	2.37527900	0.50008800	-2.18429900
H	1.61855200	0.02347400	2.00259600
H	3.21289300	-1.86263500	2.07799000
H	4.39699800	-2.57506000	0.01791600
O	-0.22796100	1.37937500	0.64612600
H	-0.75021700	0.65031900	0.24852100
C	0.94691000	1.59045600	-0.13769400
H	0.66065400	1.74950300	-1.18500300
C	1.60964700	2.86462300	0.37873800
H	1.89690500	2.74552700	1.42621900
H	2.50575200	3.09550100	-0.20007800
H	0.91755200	3.70571300	0.30021500
C	-3.99764700	0.72970600	-0.81902500
H	-3.78360500	0.92130600	-1.86885800
H	-5.07370600	0.65010400	-0.66564200
H	-3.56445700	1.50399400	-0.18713200
C	-3.64681400	-0.90791700	1.35689300
H	-4.73039000	-0.96036600	1.46007200
H	-3.18947700	-1.80732400	1.76491300
H	-3.24706600	-0.01653800	1.83851100
O	-1.72749400	-0.67164600	-0.50640100
S	-3.24018400	-0.87229500	-0.41428800



1PE-c1··DMSO (pcm DMSO) -- #2

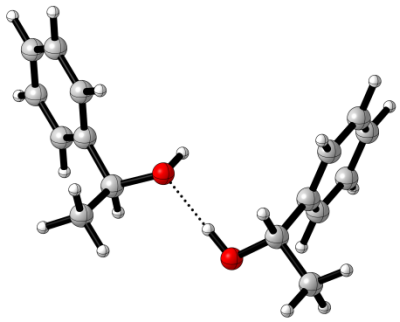
C	-2.46682400	-1.96067600	0.89647800
C	-2.12498400	-0.63669400	1.16270100
C	-1.77013700	0.23316600	0.13080800
C	-1.75660100	-0.25287300	-1.17878800
C	-2.09432800	-1.57530300	-1.44915300
C	-2.45294800	-2.43423200	-0.41210900
H	-2.73690300	-2.62236100	1.71139800
H	-2.13065600	-0.27686300	2.18651700
H	-1.47036100	0.40847000	-1.98774700
H	-2.07709600	-1.93744500	-2.47077100
H	-2.71381900	-3.46473000	-0.62261100
O	-0.34543400	2.17216100	-0.34315500
H	0.46980700	1.69747600	-0.07108400
C	-1.44279900	1.68873600	0.43116900
H	-1.19451300	1.76146500	1.49759800
C	-2.63122300	2.60464200	0.15076900
H	-2.89673100	2.56812100	-0.90856800
H	-3.50113600	2.29865000	0.73470000
H	-2.38055800	3.63489000	0.41221100
C	3.00430800	-1.40867700	1.10533600
H	2.06886600	-1.72256600	1.56449600
H	3.51100800	-2.26683000	0.66438500
H	3.64075100	-0.90117200	1.82932100
C	4.25703500	0.18122700	-0.74809200
H	4.73318300	-0.71289100	-1.14989100
H	4.16007200	0.93486000	-1.52729700
H	4.80836900	0.57411900	0.10530500
O	2.02311500	0.99789900	0.47566700
S	2.57245500	-0.24809800	-0.22267300



Dimer 1PE-c1··1PE-c1 (pcm chloroform)

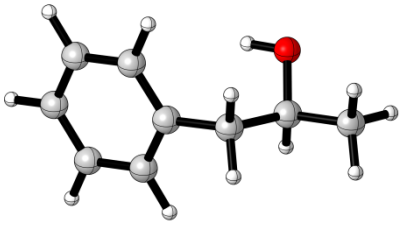
C	3.51431900	2.29701000	0.94418700
C	3.27466600	0.95025600	1.20614500
C	3.06760000	0.04403700	0.16580200
C	3.09630200	0.51609100	-1.14878000
C	3.33157500	1.86108700	-1.41466100
C	3.54375400	2.75661300	-0.36862600

H	3.67086100	2.98679100	1.76547500
H	3.24406300	0.60050400	2.23299400
H	2.92397200	-0.17575800	-1.96453600
H	3.34979500	2.21215900	-2.44012800
H	3.72553300	3.80456500	-0.57606600
O	1.83264900	-2.00473800	-0.36563800
H	0.99066600	-1.54337400	-0.19300700
C	2.84522600	-1.43118600	0.46321600
H	2.54547400	-1.51886700	1.51542300
C	4.11278900	-2.25381400	0.25274200
H	4.43343000	-2.19681900	-0.78998500
H	4.92246600	-1.88233700	0.88341100
H	3.92550400	-3.30005100	0.50280200
C	-5.02729600	0.90037600	-0.96518300
C	-3.92491100	0.08426600	-1.20616400
C	-3.03965200	-0.24067400	-0.17841100
C	-3.27181800	0.27579500	1.09925900
C	-4.36782900	1.09637900	1.34113000
C	-5.25100400	1.40891600	0.30988600
H	-5.70536200	1.14349300	-1.77475700
H	-3.75055100	-0.30251900	-2.20467700
H	-2.58619900	0.03978400	1.90446400
H	-4.53451300	1.49255700	2.33600600
H	-6.10484200	2.04847200	0.49948900
O	-0.64113300	-0.63114200	0.11996600
H	-0.52873000	0.27914300	-0.18337300
C	-1.86291100	-1.15760200	-0.44833300
H	-1.73367300	-1.24246900	-1.53258100
C	-2.04693800	-2.55113800	0.13761300
H	-2.17032400	-2.49893200	1.22118400
H	-2.93340200	-3.02308800	-0.28880400
H	-1.17952100	-3.17467100	-0.08690300



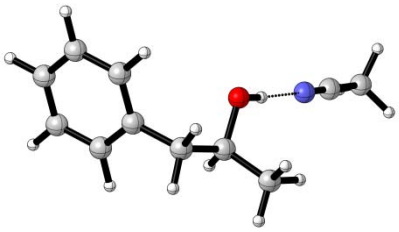
1P2P-c1 (pcm chloroform)

C	3.04681000	0.06088100	0.32164400
C	2.36794100	1.16817600	-0.17522300
C	1.03792400	1.05240000	-0.57419100
C	0.36285400	-0.16812100	-0.48294400
C	1.06014600	-1.27354000	0.01678900
C	2.38778700	-1.16288500	0.41487800
H	4.08216900	0.14757000	0.62898300
H	2.87302400	2.12348800	-0.25796800
H	0.52056700	1.91875100	-0.97172900
H	0.55881000	-2.23314800	0.08763500
H	2.91068700	-2.03320000	0.79410400
C	-1.09045500	-0.28662600	-0.87693000
H	-1.26121100	-1.24688300	-1.37234700
H	-1.35105300	0.50011800	-1.59040600
C	-2.05679200	-0.19322300	0.31826000
H	-1.80929200	-0.99335000	1.02822200
C	-3.50782200	-0.33524900	-0.10679300
H	-3.67500700	-1.30379100	-0.58229400
H	-4.16715700	-0.25819700	0.75942000
H	-3.77794600	0.45088900	-0.81611200
O	-1.94161600	1.07061000	0.98823000
H	-1.02101600	1.19199700	1.25370300



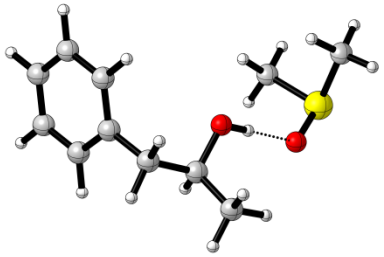
1P2P-c2··ACN (pcm ACN)
(lowest energy structure)

C	-3.70255600	-1.77333900	0.11865700
C	-3.22568900	-1.18808600	1.28932600
C	-2.39543900	-0.07321300	1.22526300
C	-2.02092500	0.47803400	-0.00448000
C	-2.51002100	-0.11693400	-1.16941900
C	-3.34278100	-1.23200000	-1.11197700
H	-4.35175300	-2.63967100	0.16622600
H	-3.50503200	-1.59708400	2.25354300
H	-2.03753400	0.37882700	2.14454200
H	-2.23644300	0.29821900	-2.13309600
H	-3.71094600	-1.67668100	-2.02944100
C	-1.11073900	1.68240400	-0.06172400
H	-1.43439800	2.41859100	0.67956800
H	-1.18703300	2.16047200	-1.04270200
C	0.36816000	1.37548100	0.20329600
H	0.44518500	0.83347000	1.15501500
C	1.19998400	2.65231900	0.29172700
H	0.86558900	3.27763400	1.12357100
H	2.25399400	2.41391900	0.45094700
H	1.11474800	3.22965900	-0.63271200
O	0.83323000	0.52898500	-0.85388400
H	1.72077700	0.20353800	-0.62539200
C	4.55670500	-1.00229700	-0.02067200
N	3.51181100	-0.56848100	-0.22389800
C	5.87855700	-1.55005400	0.23689500
H	6.53761000	-0.76455900	0.60776200
H	5.81102400	-2.34227800	0.98302200
H	6.29416400	-1.96046300	-0.68383900



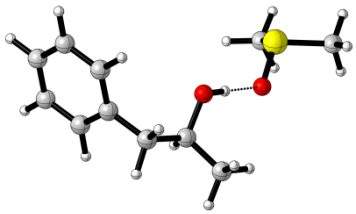
1P2P-c2··DMSO (pcm DMSO)

C	3.84488600	-2.04943800	-0.11917100
C	3.71458400	-1.19407800	-1.21078400
C	3.08748200	0.03922700	-1.06107800
C	2.57489100	0.44343700	0.17603100
C	2.71665800	-0.42310700	1.26228600
C	3.34474100	-1.65810400	1.11941600
H	4.33599500	-3.00874800	-0.23232700
H	4.10679000	-1.48512100	-2.17852400
H	2.99982500	0.70044500	-1.91700400
H	2.33176900	-0.12715800	2.23190100
H	3.44441900	-2.31367200	1.97695900
C	1.88522200	1.77943900	0.32154900
H	2.44994300	2.54072400	-0.22405300
H	1.87339800	2.08067300	1.37322500
C	0.44108900	1.80895200	-0.19596200
H	0.43584000	1.43279200	-1.22789400
C	-0.12895500	3.22551700	-0.18552900
H	0.44259800	3.88110200	-0.84779400
H	-1.16694300	3.22221300	-0.52534300
H	-0.10004500	3.64268800	0.82474100
O	-0.33669700	0.93379000	0.62401100
H	-1.21666100	0.81304500	0.21042300
S	-3.81476800	-0.56349000	-0.43840900
O	-2.83716800	0.60200300	-0.58625500
C	-2.85086900	-2.08223000	-0.69945900
H	-3.49876000	-2.93730000	-0.50784100
H	-2.53631000	-2.07892600	-1.74137400
H	-1.98871000	-2.08249300	-0.03384900
C	-4.11800200	-0.75594600	1.34350900
H	-4.65261100	0.13480700	1.66818000
H	-4.73811100	-1.63943500	1.49425100
H	-3.16557000	-0.84813800	1.86397700



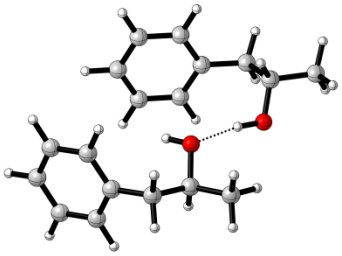
1P2P-c2··DMSO (pcm DMSO) -- #2

```
C  4.09290500   -2.04818800    0.01001100
C  3.85541600   -1.34386900   -1.16807600
C  3.20026700   -0.11674100   -1.12848500
C  2.76565600    0.43116800    0.08289900
C  3.01476500   -0.28445700    1.25621900
C  3.67138100   -1.51243600    1.22350900
H  4.60589200   -3.00230500   -0.01784300
H  4.18567300   -1.74788600   -2.11821300
H  3.02891200    0.42651400   -2.05209400
H  2.69202700    0.12504600    2.20699400
H  3.85462100   -2.04959500    2.14706300
C  2.04401800    1.75779900    0.11051800
H  2.54580400    2.45828900   -0.56305800
H  2.09272000    2.18782300    1.11534100
C  0.56860500    1.68696600   -0.30435600
H  0.50822700    1.18951300   -1.28190000
C -0.04733900    3.07924900   -0.42229300
H  0.45826000    3.66568100   -1.19399600
H -1.10417200    3.00820800   -0.68873600
H  0.03171500    3.61474200    0.52773200
O -0.12304600    0.89710000    0.66521300
H -1.02738800    0.71434900    0.33368300
S -3.49160100   -0.76832200    0.32604700
O -2.67844300    0.36161700   -0.30833500
C -5.15406100   -0.08887100    0.59531400
H -5.80587400   -0.89271100    0.93669400
H -5.06153700    0.67136600    1.36860100
H -5.51556700    0.34634100   -0.33568000
C -3.89827700   -1.91070600   -1.02639200
H -2.96259600   -2.36595600   -1.34535600
H -4.57412300   -2.67481200   -0.64268500
H -4.35507300   -1.35067500   -1.84152100
```



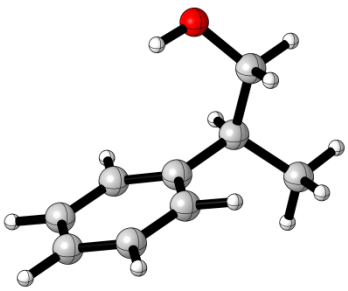
Dimer 1P2P-c1··1P2P-c1 (pcm chloroform)

```
C  4.36826400    1.41958200    0.35274000
C  3.71908900    1.29823800   -0.87092000
C  3.03136400    0.12817400   -1.18519900
C  2.98082500   -0.93968600   -0.28608800
C  3.63937800   -0.80343700    0.94115500
C  4.32589900    0.36290800    1.25965400
H  4.90734600    2.32703800    0.59767700
H  3.74960200    2.11243200   -1.58556700
H  2.53465400    0.03981500   -2.14514200
H  3.62232700   -1.62387300    1.65100900
H  4.83423200    0.44545500    2.21332500
C  2.22452800   -2.20467800   -0.61869000
H  2.81099800   -3.07405000   -0.30664800
H  2.08143700   -2.28163400   -1.69993700
C  0.84738300   -2.30925800    0.05646300
H  0.97692800   -2.22685700    1.14220300
C  0.15161100   -3.61942900   -0.26932000
H  0.75171400   -4.46261700    0.07794900
H -0.82453400   -3.66768800    0.21499600
H  0.00728800   -3.71861900   -1.34801700
O -0.02848300   -1.24941000   -0.38027800
H  0.36046700   -0.39706700   -0.14005000
C -0.08641900    2.92269100   -0.14236200
C -0.32750400    2.26361400    1.05977300
C -1.51569300    1.56101600    1.24671200
C -2.48257200    1.50053900    0.23954000
C -2.22726500    2.17106600   -0.96092800
C -1.04309500    2.87547300   -1.15294700
H  0.83632000    3.47117100   -0.28809000
H  0.40797600    2.29967300    1.85514100
H -1.69693600    1.05448800    2.18803100
H -2.96796000    2.14555300   -1.75352800
H -0.86863100    3.39064600   -2.09054600
C -3.75606600    0.71341800    0.42488900
H -4.58215300    1.23860000   -0.06419800
H -4.00066400    0.64131200    1.48852300
C -3.70048600   -0.72014500   -0.14401400
H -3.42879900   -0.66176600   -1.20591700
C -5.04683200   -1.41768400   -0.01413700
H -5.82713700   -0.86114100   -0.53771200
H -4.99531200   -2.42297400   -0.43581300
H -5.33091900   -1.50224300    1.03821100
O -2.73783300   -1.52046600    0.54298000
H -1.84216800   -1.32105500    0.21455700
```



2P1P-c1 (pcm chloroform)

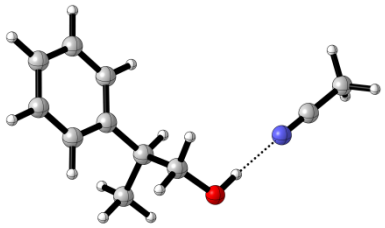
```
C -2.84601800   -0.07670400   -0.22484700
C -2.27237300   -0.68903000    0.88389400
C -0.90481400   -0.56702000    1.11966800
C -0.08498100    0.16750000    0.25949400
C -0.67716700    0.77565000   -0.85371400
C -2.04172500    0.65617800   -1.09425700
H -3.90932100   -0.16876400   -0.41167300
H -2.88712100   -1.26302200    1.56744700
H -0.46649000   -1.04836500    1.98720300
H -0.07012900    1.35256900   -1.54231200
H -2.47853500    1.13714500   -1.96179400
C  1.40724200    0.28183100    0.52724100
H  1.60768400   -0.22094400    1.47829900
C  1.87971600    1.73914600    0.64850900
H  1.32203500    2.26399400    1.42614400
H  2.94075000    1.77886000    0.90705800
H  1.74393000    2.28704200   -0.28698700
C  2.23110400   -0.45143600   -0.54201100
H  2.07609600    0.01473000   -1.52299800
H  3.29269300   -0.37254100   -0.30141100
O  1.95764300   -1.85118400   -0.60867300
H  1.02136100   -1.96792200   -0.81345400
```



2P1P-c8··ACN (pcm ACN)
(lowest energy structure)

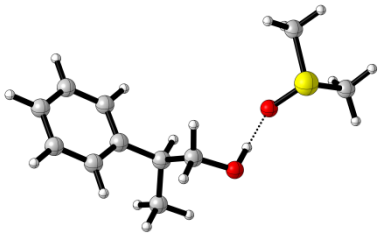
```
C  3.87480900    1.53031800   -0.29925100
C  3.87890400    0.16237900   -0.56026400
C  2.74553500   -0.60412700   -0.30561500
C  1.58287800   -0.02265500    0.21333800
```

C	1.59408300	1.35182400	0.46638500
C	2.72642100	2.12314600	0.21635100
H	4.75813000	2.12669900	-0.49472200
H	4.76771000	-0.31043700	-0.96204200
H	2.77370700	-1.66785500	-0.51213500
H	0.70399700	1.82441600	0.86806300
H	2.71024600	3.18656200	0.42561200
C	0.33236600	-0.84359000	0.47517500
H	-0.39980700	-0.17748500	0.94393500
C	0.57744100	-2.02191200	1.42773800
H	0.95902800	-1.67280600	2.38969200
H	-0.35230200	-2.56476800	1.60363100
H	1.30281400	-2.72672600	1.01335500
C	-0.28355400	-1.31232600	-0.85875600
H	-0.39707500	-0.45276600	-1.52914100
H	0.38807800	-2.02385900	-1.34608200
O	-1.53010600	-1.98394500	-0.69921400
H	-2.21766100	-1.32295900	-0.50758100
C	-4.55767000	0.70658200	-0.07824900
N	-3.68595400	-0.02861400	-0.22237400
C	-5.66021000	1.63644500	0.10419600
H	-5.28718200	2.66070800	0.07909100
H	-6.39173500	1.50239900	-0.69316200
H	-6.14144800	1.45423400	1.06553600



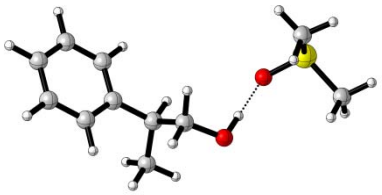
2P1P-c2··DMSO (pcm DMSO) -- #1

C	4.69648000	1.52385200	-0.20783700
C	3.60888500	2.01514900	0.50766000
C	2.49109700	1.21161100	0.71906800
C	2.43449900	-0.09570000	0.22787600
C	3.53646800	-0.57522900	-0.48978900
C	4.65481100	0.22427500	-0.70671900
H	5.56822400	2.14556900	-0.37425700
H	3.62895900	3.02421300	0.90305300
H	1.64858900	1.60493700	1.27803500
H	3.52823400	-1.58526300	-0.88316000
H	5.49617400	-0.16938900	-1.26542600
C	1.19868700	-0.94949600	0.44999900
H	0.52399800	-0.38087600	1.09871000
C	1.50817400	-2.28354400	1.14304500
H	1.98337400	-2.11868600	2.11259600
H	0.58818900	-2.84767000	1.30298400
H	2.17858500	-2.90138300	0.54000400
C	0.45433800	-1.16325200	-0.88458600
H	0.29466800	-0.19175300	-1.36766600
H	1.07116700	-1.76648700	-1.55663100
O	-0.77990800	-1.85406900	-0.73845400
H	-1.43485700	-1.24609500	-0.33317200
S	-3.83173700	0.29382100	-0.42381800
O	-2.64156700	-0.16309800	0.42319600
C	-5.31462900	-0.13346300	0.53342900
H	-6.18607500	0.27572600	0.02266100
H	-5.37115800	-1.22009700	0.55624200
H	-5.21872900	0.27106600	1.54035500
C	-3.91214200	2.09803800	-0.23341800
H	-3.03117800	2.50537500	-0.72584600
H	-4.81555900	2.45810400	-0.72516700
H	-3.91301900	2.34545600	0.82745500



2P1P-c2··DMSO (pcm DMSO) -- #2

C	4.75541300	-1.35849700	0.22124000
C	3.77457900	-1.81729800	-0.65266400
C	2.61908200	-1.06829900	-0.86148800
C	2.41831300	0.15189600	-0.21002500
C	3.41405600	0.59964400	0.66596300
C	4.56930500	-0.14616100	0.88085900
H	5.65614900	-1.93785000	0.38611700
H	3.90755000	-2.75832300	-1.17394600
H	1.86071800	-1.43572500	-1.54476900
H	3.29308700	1.54275200	1.18642200
H	5.32651800	0.22149700	1.56384700
C	1.14257700	0.94425000	-0.43452600
H	0.57408600	0.42891200	-1.21590100
C	1.40485700	2.38004100	-0.90934100
H	1.97612400	2.38488700	-1.84028200
H	0.46100300	2.89852500	-1.08347000
H	1.96746500	2.95067200	-0.16591400
C	0.27110300	0.91799200	0.83853000
H	0.14999200	-0.11963500	1.17155500
H	0.77633000	1.46336800	1.64057000
O	-0.99889200	1.53529600	0.66681600
H	-1.57190500	0.93660100	0.14273900
S	-3.94960600	-0.77336000	-0.46123500
O	-2.61191900	-0.14636800	-0.85566600
C	-3.67716900	-1.60764800	1.13043000
H	-4.63482300	-1.98365900	1.48997100
H	-2.99938400	-2.43714800	0.93769500
H	-3.23864700	-0.90381200	1.83669500
C	-4.99698600	0.58563600	0.13832400
H	-5.20099600	1.22564500	-0.71800700
H	-5.92653700	0.16164900	0.51756800
H	-4.46734600	1.13464100	0.91585500



Dimer 2P1P-c1··2P1P-c1 (pcm chloroform)

C	-3.83961400	2.17914500	-0.37141600
C	-3.52269000	1.48479600	-1.53381700
C	-3.08044400	0.16602300	-1.46094100
C	-2.94891500	-0.48565300	-0.23271800
C	-3.26802500	0.22752000	0.92838100
C	-3.70868800	1.54492700	0.86152100
H	-4.18560400	3.20465000	-0.42380200
H	-3.61949300	1.96737500	-2.49947300
H	-2.83638600	-0.36771300	-2.37310400
H	-3.17690100	-0.24802900	1.89855400
H	-3.95262100	2.07689300	1.77383700
C	-2.47562400	-1.92889800	-0.17295900
H	-2.33448000	-2.27030700	-1.20284700
C	-3.50077500	-2.85646200	0.50019800
H	-4.46670800	-2.79421300	-0.00381600
H	-3.16400900	-3.89532500	0.46171400
H	-3.65468900	-2.59372400	1.54949800
C	-1.11550700	-2.06594300	0.52365300
H	-1.17384500	-1.71584700	1.55991800
H	-0.82121200	-3.11626600	0.54213600
O	-0.05834700	-1.38840400	-0.16710400
H	-0.18320900	-0.43242700	-0.09439300
C	0.73956100	2.45926700	0.59903300
C	1.45459400	1.96847000	1.68651900
C	2.50934700	1.08118400	1.48622400
C	2.87484000	0.66762900	0.20358400
C	2.15085800	1.17512700	-0.88100800
C	1.09363200	2.05910700	-0.68803200
H	-0.08509200	3.14543100	0.74949600
H	1.19013300	2.27203000	2.69289300
H	3.05491400	0.69740400	2.34141700
H	2.40646300	0.87384700	-1.89071000
H	0.54470300	2.43630500	-1.54302600
C	4.01197300	-0.31882800	0.00615200
H	4.42582000	-0.54048500	0.99474900
C	5.14100800	0.25182600	-0.86720500
H	5.52861700	1.18103500	-0.44536600

H	5.96863000	-0.45843100	-0.93915500
H	4.79611100	0.46532400	-1.88201400
C	3.52402800	-1.65938800	-0.57323300
H	3.10069700	-1.50373400	-1.57349600
H	4.38445400	-2.32427700	-0.68448200
O	2.59649400	-2.33804600	0.26264500
H	1.71117600	-1.94698500	0.14352900