Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The Evolution Towards Cyclic Structures in the Aggregation of Aromatic Alcohols: The Dimer, Trimer and Tetramer of 2-Phenylethanol†

ELECTRONIC SUPPLEMENTARY INFORMATION

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DFT calculations were implemented in gaussian16, including the geometry optimization and frequency calculations. The vibrational modes were obtained using the double-harmonic approximation. The B3LYP functional was supplemented with D3 empirical dispersion corrections and the Becke-Johnson dumpling function.

At the B3LYP-D3(BJ)/def2TZVP, a correction factor of 0.963 was used to account for the anharmonicity of wavenumber values of both CH and OH stretching modes. In order to reproduce the bandwidth observed in the experimental vibrational spectrum, first, each frequency was represented with a Lorentzian function with a FWMH of 5 cm^{-1}. Then, the effect of the laser on the shape of the transition was also taken into account by the convolution of a Gaussian function (FWMH = 6 cm^{-1}). Finally, to simulate the band broadening of the stretching vibrations of polar groups due to hydrogen bond formation, the FWMH of the bands involved in the interactions was adjusted to 10 cm^{-1} for those OH vibrational modes down to 3550 cm^{-1}, of 15 cm^{-1} for those modes between 3400-3550 cm^{-1} and of 40 cm^{-1} for those bellow 3400 cm^{-1}. Complexation energies were corrected for the BSSE, using the counterpoise approximation.

Gaussian16 keywords for the B3LYP-D3(BJ)/def2TZVP calculation

```
# B3LYP EmpiricalDispersion=GD3BJ def2TZVP Integral(Grid=UltraFineGrid) opt=tight
freq density=current output=pickett prop=EFG
# B3LYP EmpiricalDispersion=GD3BJ def2TZVP counterpoise=2 density=current
output=pickett prop=EFG
```

1. Supplementary Figures

Figure S1. A) Comparison between the 2c-REMPI spectrum of PhEtOH and the UV/UV hole burning traces obtained probing the bands at 37627 cm^{-1} (Isomer Ggπ) and 37675 cm^{-1} (Isomer At); B) comparison between the IR/UV spectra obtained probing the same UV transitions as in the hole burning and the simulations obtained using normal mode analysis (red traces) and anharmonic calculations (blue trace). A correction factor of 0.963 was used for the harmonic simulation.

Figure S2. Microwave spectrum of PhEthOH in the region 2-8 GHz. The positive trace (blue) is the original spectrum, including the monomer, isotopic satellites, possible clusters and impurities. The negative (red) trace spectrum corresponds to the subtraction of the monomer's transitions.

Figure S3. a) 2c-REMPI spectrum of PhEtOH dimer, along with the UV/UV hole burning spectra obtained tuning the "burning" laser at b) 37460 cm^{-1} (red asterisk), c) 37493 cm^{-1} (blue asterisk) and d) 37474 cm^{-1} (green asterisk). Ionization wavelength was set to 35714 cm^{-1}. e) IR/UV spectra of PhEtOH dimer. Roman numbers mark the transitions probed to obtain each IR spectrum.

Figure S4. IR/UV hole burning spectra obtained for PhEtOH dimer.

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Figure S6. Computed higher-energy structures of the PhEtOH dimer at B3LYP-D3(BJ)/def2TZVP level. Energies inside brackets are given in kJ/mol.

Figure S7. Some selected additional structures of the PhEtOH trimer as computed at B3LYP-D3(BJ)/def2TZVP level. Energies inside brackets are given in kJ/mol.

Figure S8. Some selected additional structures of the PhEtOH tetramer as computed at B3LYP-D3(BJ)/def2TZVP level. Energies inside brackets are given in kJ/mol.

3. Supplementary Tables

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Table S2. Comparison of the experimental parameters of 2-phenylethanol dimer with the predictions using the B3LYP-D3(BJ) method and a polarized triple-ζ basis set (def2-TZVP), together with the main structural parameters of the hydrogen bond.

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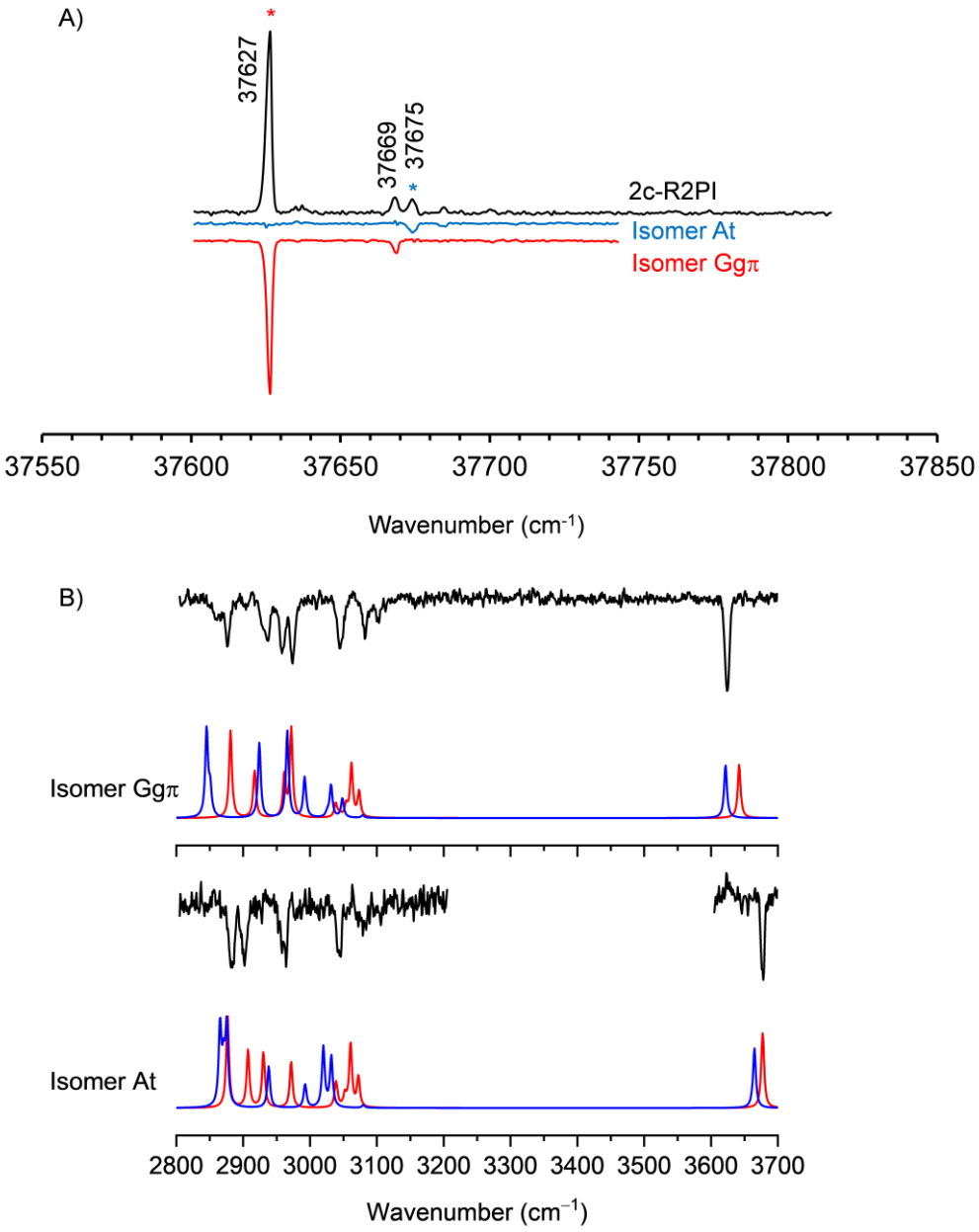

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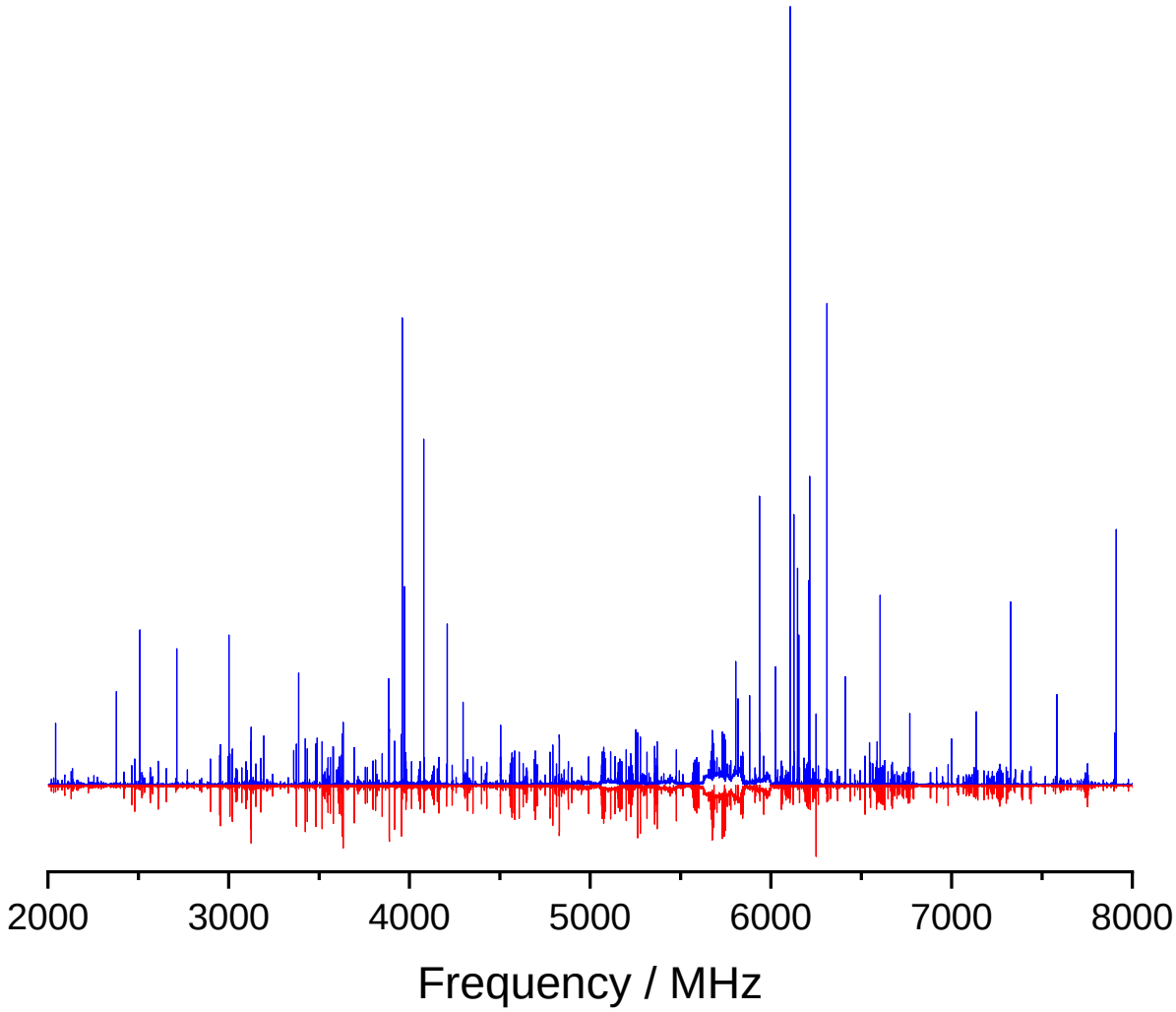

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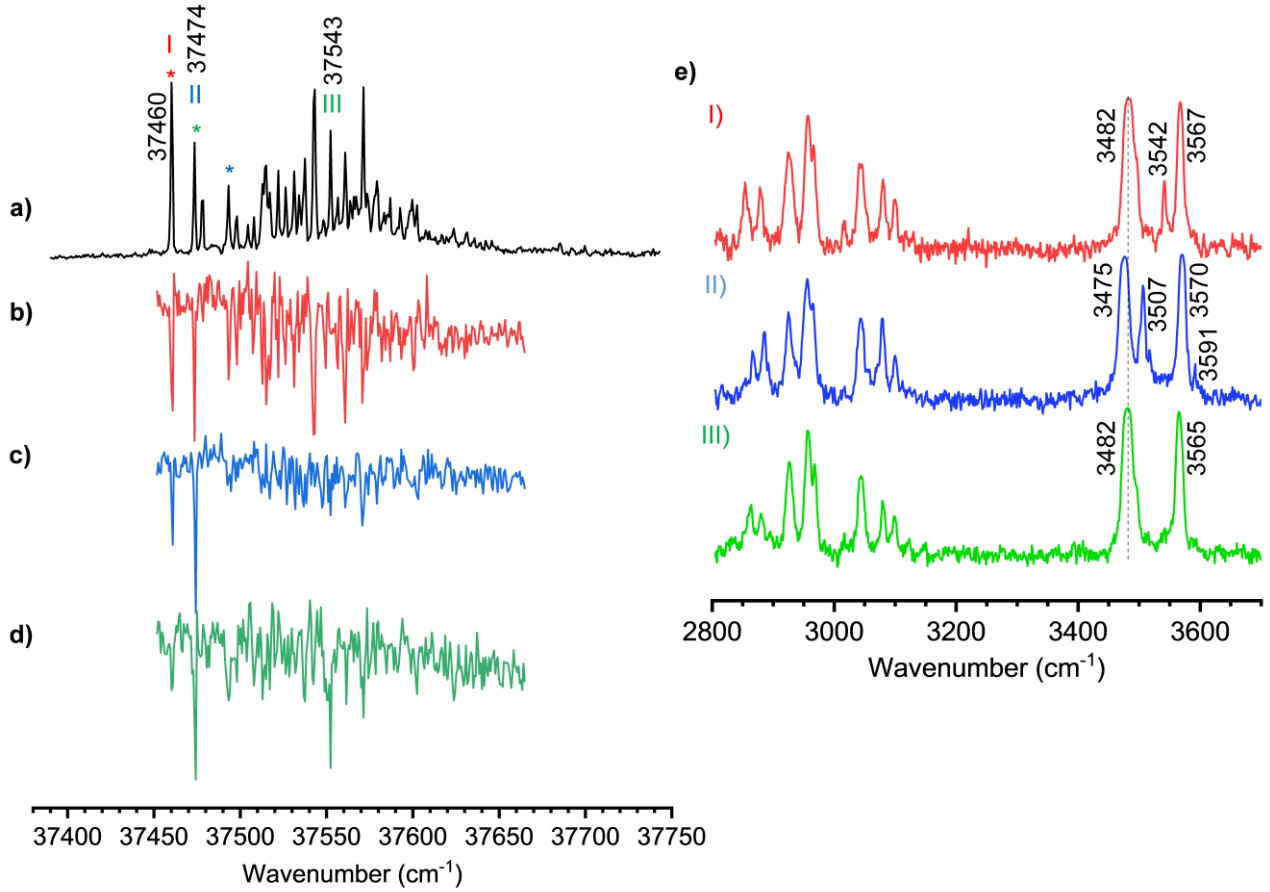


Figure S4. IR/UV hole burning spectra obtained for PhEtOH dimer.

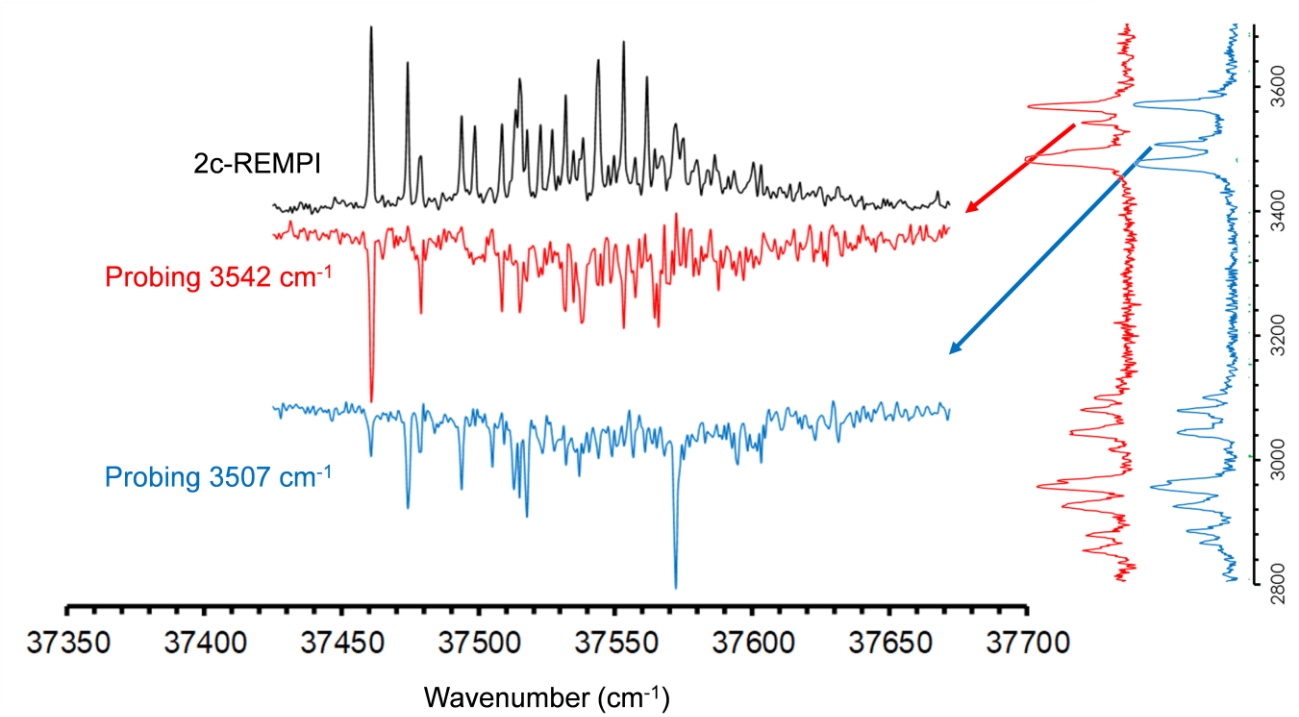


Figure S5. Comparison between the experimental IR/UV spectra of the three isomers of PhEtOH dimer and the simulations using the computations at B3LYP-D3(BJ)/def2TZVP level (red), B2PLYP-D3(BJ)/def2TZVP (blue) and MP2/def2TZVP (green trace). Visual inspection shows that the predictions at B3LYP-D3(BJ)/def2TZVP level better reproduce the experimental results and therefore, this is the computation level used for the assignment of the rest of the IR/UV spectra.

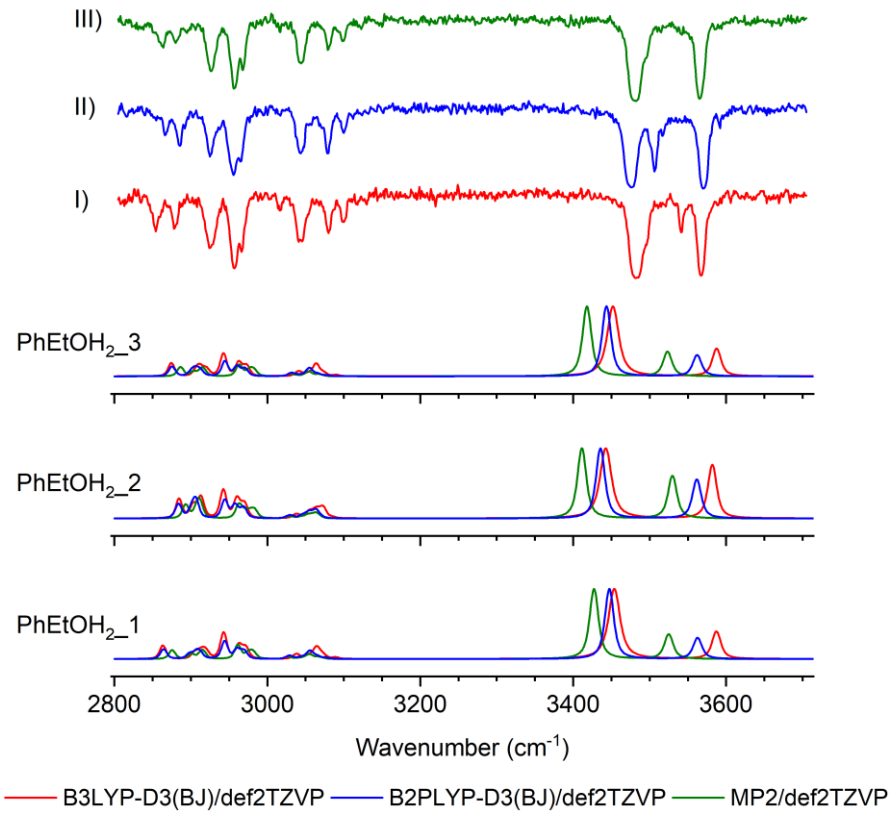
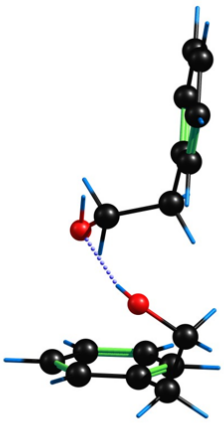


Figure S6. Computed higher-energy structures of the PhEtOH dimer at B3LYP-D3(BJ)/def2TZVP level. Energies inside brackets are given in kJ/mol.



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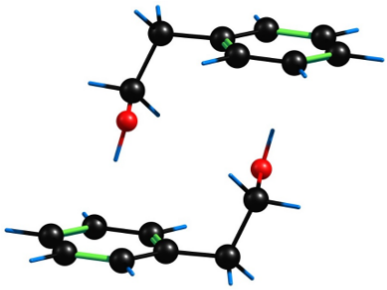
(Ggπ- Ggπ+ Lp+)
$[10.6]_{0K}$ $[9.1]_{298K}$



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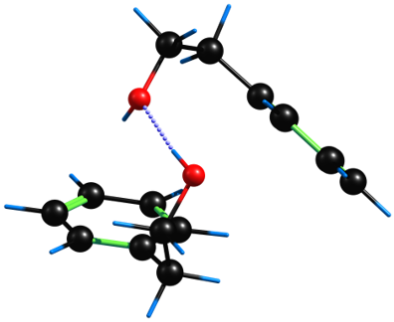
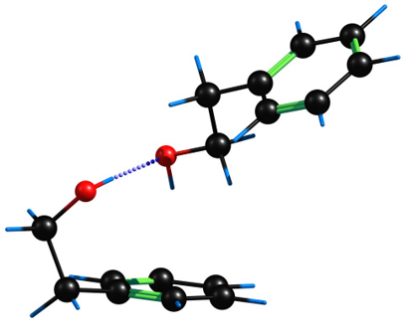
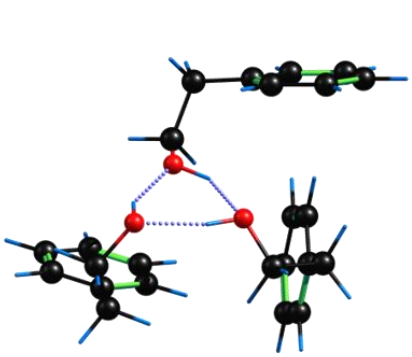


$PhEtOH_2$_07
(Ggπ+ Gπ- Lp-)
$[8.7]_{0K}$ $[9.3]_{298K}$



$PhEtOH_2$_08
(Ggπ+ At Lp-)
$[10.1]_{0K}$ $[5.6]_{298K}$

Figure S7. Some selected additional structures of the PhEtOH trimer as computed at B3LYP-D3(BJ)/def2TZVP level. Energies inside brackets are given in kJ/mol.



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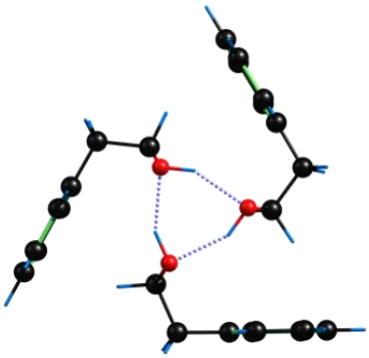
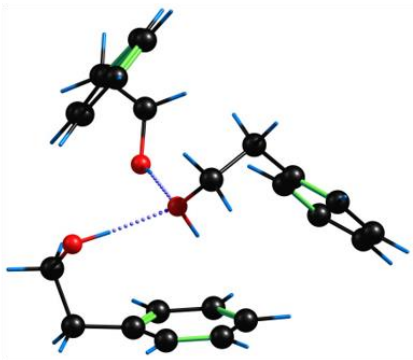
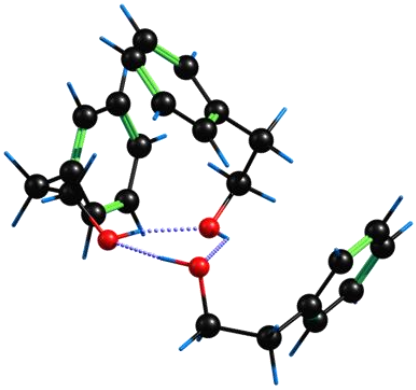
(E Ggπ+ Ggπ-)
$[7.9]_{0K}$ $[4.6]_{298K}$



$PhEtOH_3$_10
(Gg+ Gg+ Gg+)
$[12.7]_{0K}$ $[11.0]_{298K}$

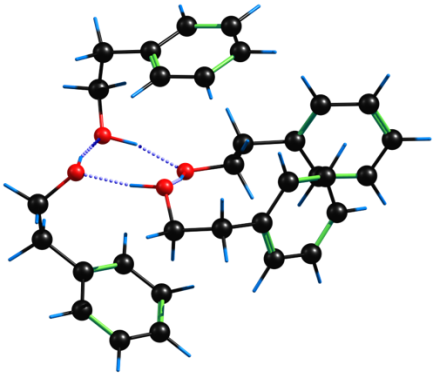


$PhEtOH_3$_07
(Ggπ+ Lp+ Ggπ- Lp- Ggπ+)
$[5.6]_{0K}$ $[4.3]_{298K}$

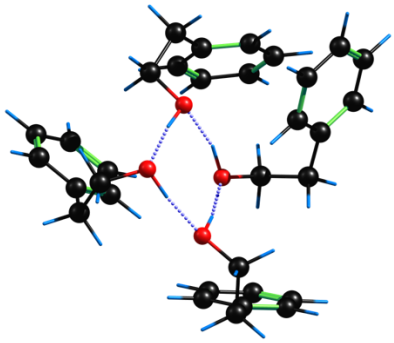


$PhEtOH_3$_08
(Gt Gt Ggπ+)
$[6.5]_{0K}$ $[3.4]_{298K}$

Figure S8. Some selected additional structures of the PhEtOH tetramer as computed at B3LYP-D3(BJ)/def2TZVP level. Energies inside brackets are given in kJ/mol.



PhEtOH$_4$_09
(Gg- At Gt Gg-)
$[6.3]_{0K}$ $[0.5]_{298K}$



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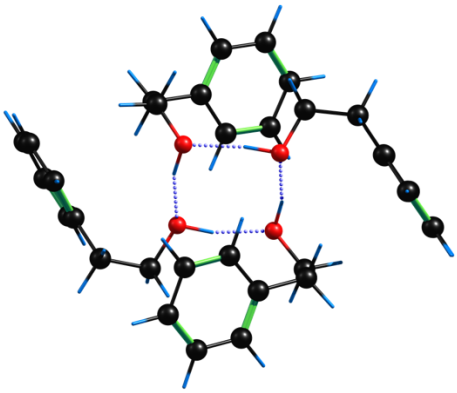
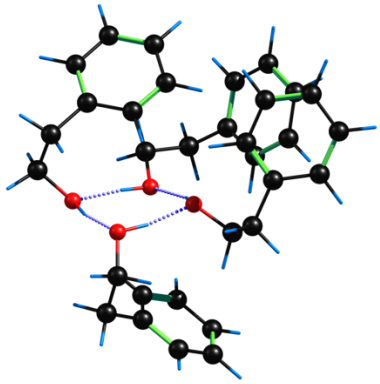
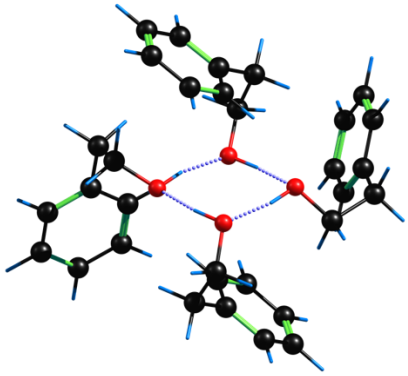
(Gg+ Gg- Gg+ Gt)
$[7.0]_{0K}$ $[3.9]_{298K}$



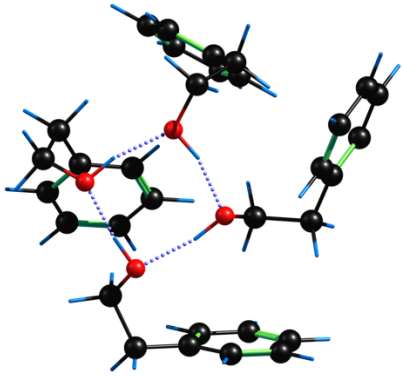
PhEtOH$_4$_07
(Gt Gg+ Gt Gg-)
$[5.8]_{0K}$ $[4.9]_{298K}$



PhEtOH$_4$_08
(Gg- Gt Gt Gg-)
$[5.8]_{0K}$ $[7.1]_{298K}$



PhEtOH$_4$_05
(Gg- Gg+ Gt Gg-)
$[5.5]_{0K}$ $[3.5]_{298K}$



PhEtOH$_4$_06
(Gg- Gg+ Gt Gg-)
$[5.6]_{0K}$ $[7.3]_{298K}$

1. Supplementary Tables

Table S1. Prediction of the rotational and energetic parameters for 2-phenylethanol dimer using the B3LYP-D3(BJ) method and a polarized triple-ζ basis set (def2-TZVP).

Isomer	(PhEtOH)2_01	(PhEtOH)2_02	(PhEtOH)2_03	(PhEtOH)2_04	(PhEtOH)2_05
	Ggπ+Ggπ-Lp-	Ggπ+Ggπ-Lp+	Ggπ-Ggπ− Lp-	Ggπ-Gt Lp-	Ggπ+Ggπ-Lp+
A / MHz [a]	717.62	563.87	724.81	563.75	606.63
B / MHz	280.79	317.79	274.57	317.92	321.97
C / MHz	241.99	288.68	236.49	288.73	289.01
D_J / kHz [b]	0.0187	0.0338	0.0111	0.0249	0.0303
D_{JK} / kHz	-0.0450	0.0056	-0.0055	0.1154	0.1116
D_K / kHz	0.1946	0.0130	0.1211	-0.0829	-0.1146
d_1 / kHz	-0.0040	0.0013	-0.0017	-0.0025	0.0019
d_2 / kHz	0.0000	-0.0009	-0.0001	-0.0019	-0.0022
$\lvert\mu_a\rvert$ / D	2.34	0.69	2.25	0.70	0.61
$\lvert\mu_b\rvert$ / D	1.02	1.37	1.33	1.36	1.73
$\lvert\mu_c\rvert$ / D	1.95	1.30	0.08	1.30	2.23
ΔE_{ZPE} / kJ mol^{-1} [c]	0.00	0.13	0.64	6.09	7.13
ΔG / kJ mol^{-1}	0.00	0.88	1.38	7.02	8.18
Ec / kJ mol^{-1}	-53.2	-55.5	-53.9	-59.8	-48.2

[a]Rotational constants (A, B, C). [b]Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2) and electric dipole moments (μ_α, α = a, b, c). [c]Relative energy with zero-point corrections (ΔE), Gibbs energy (ΔG, 298K, 1 atm) and complexation energy (ΔE_c including BSSE corrections).

Table S1. Continued.

Isomer	(PhEtOH)2_06	(PhEtOH)2_07	(PhEtOH)2_08	(PhEtOH)2_09
	Ggπ-Ggπ-Lp-	Ggπ+Gπ-Lp+	Ggπ+At Lp-	Ggπ-Ggπ+ Lp+
A / MHz [a]	545.14	529.61	718.51	755.24
B / MHz	318.15	345.65	200.94	227.81
C / MHz	241.88	318.60	187.13	199.15
D_J / kHz [b]	0.0449	0.0483	0.0220	0.0195
D_{JK} / kHz	0.0022	0.0132	0.2759	-0.0545
D_K / kHz	0.0959	-0.0256	0.1637	0.2181
d_1 / kHz	-0.0067	-0.0031	0.0012	-0.0023
d_2 / kHz	-0.0029	-0.0004	0.0002	-0.0000
$\lvert\mu_a\rvert$ / D	2.23	0.05	0.00	0.67
$\lvert\mu_b\rvert$ / D	1.44	2.30	2.06	1.88
$\lvert\mu_c\rvert$ / D	0.51	0.45	2.11	1.19
ΔE_{ZPE} / kJ mol^{-1} [d]	8.09	8.65	10.08	10.58
ΔG / kJ mol^{-1}	5.06	9.29	5.58	9.11
Ec / kJ mol^{-1}		-57.4	-48.3	

[a]Rotational constants (A, B, C). [b]Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2) and electric dipole moments (μ_α, α = a, b, c). [c]Relative energy with zero-point corrections (ΔE), Gibbs energy (ΔG, 298K, 1 atm) and complexation energy (ΔE_c including BSSE corrections).

Table S1. Continued.

Isomer	(PhEtOH)2_10	(PhEtOH)2_11
	Gt Gt	Ggπ-Ggπ-
A / MHz [a]	739.46	480.13
B / MHz	188.66	378.80
C / MHz	173.80	329.15
D_J / kHz [b]	0.0211	0.0636
D_{JK} / kHz	0.4625	0.4786
D_K / kHz	0.2009	-0.2275
d_1 / kHz	0.0048	0.0358
d_2 / kHz	-0.0001	-0.0207
$\lvert\mu_a\rvert$ / D	1.11	0.01
$\lvert\mu_b\rvert$ / D	2.05	1.06
$\lvert\mu_c\rvert$ / D	0.50	0.00
ΔE_{ZPE} / kJ mol^{-1} [d]	11.48	14.57
ΔG / kJ mol^{-1}	5.19	9.19
Ec / kJ mol^{-1}	-48.5	-33.9

[a]Rotational constants (A, B, C). [b]Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2) and electric dipole moments (μ_α, α = a, b, c). [c]Relative energy with zero-point corrections (ΔE), Gibbs energy (ΔG, 298K, 1 atm) and complexation energy (ΔE_c including BSSE corrections).

Table S2. Comparison of the experimental parameters of 2-phenylethanol dimer with the predictions using the B3LYP-D3(BJ) method and a polarized triple-ζ basis set (def2-TZVP), together with the main structural parameters of the hydrogen bond.

	Experiment			Theory		
	I	II	III	(PhEthOH)2_01 = Ggπ+Ggπ-Lp-	(PhEthOH)2_02 = Ggπ+Ggπ-Lp+	(PhEthOH)2_03 = Ggπ-Ggπ-Lp-
A / MHz [a]	708.07951(20)	563.05177(29)	713.30267(39)	717.6	563.9	724.8
B / MHz	276.410756(99)	313.31209(20)	271.81195(16)	280.8	317.8	274.6
C / MHz	237.62572(10)	286.68383(24)	233.31321(16)	242.0	288.7	236.5
D_J / kHz	0.02024(26)	0.0415(11)	0.01339(37)	0.019	0.034	0.011
D_{JK} / kHz	-0.04231(88)	[0.]	-0.0068(14)	-0.045	0.006	-0.006
D_K / kHz	0.1948(29)	0.0187(30)	0.1498(84)	0.195	0.013	0.121
d_1 / kHz	-0.00434(16)	[0.]	-0.00212(29)	-0.004	0.001	-0.002
d_2 / kHz	[0.]	[0.]	[0.]	0.0	-0.001	0.0
σ / kHz [b]	9.8	10.6	12.6			
N	438	193	310			
ΔE_{ZPE} / kJ mol^{-1}				0.0	0.1	0.6
ΔG / kJ mol^{-1}				0.0	0.9	1.4
Ec / kJ mol^{-1}				-53.2	-55.5	-53.9
Hydrogen Bond Donor [b]						
τ (HO-$C_\beta C_\alpha$) /deg				77.6	83.8	-80.2
τ (OC_β-$C_\alpha C_{ipso}$) /deg				-63.2	-61.5	59.6
τ ($C_\beta C_\alpha$-$C_{ipso}C_{ortho}$) /deg				-80.5	-82.6	76.2
Hydrogen Bond Acceptor						
τ (HO-$C_\beta C_\alpha$) /deg				-73.5	-78.4	-74.3
τ (OC_β-$C_\alpha C_{ipso}$) /deg				63.3	62.2	64.7
τ ($C_\beta C_\alpha$-$C_{ipso}C_{ortho}$)/deg				85.3	72.5	88.2
r (O-H···O) / Å				1.879	1.856	1.881
∠ (O-H···O) / deg				173.7	174.4	179.0
r (O-H···centroid) / Å				2.411	2.380	2.357
r (C-H···centroid) / Å				2.890	2.932	2.785

[a]Parameter definition as in Table S1. [b]Structural parameters of the hydrogen bond.

Table S3. Prediction of the rotational and energetic parameters for 2-phenylethanol dimer using the B2PLYP-D3(BJ) method and a polarized triple-ζ basis set (def2-TZVP).

Isomer	(PhEthOH)2_01	(PhEthOH)2_02	(PhEthOH)2_03
	Ggπ+Ggπ-Lp-	Ggπ+Ggπ-Lp+	Ggπ-Ggπ-Lp-
A / MHz [a]	718.18	565.28	724.45
B / MHz	279.97	318.05	274.73
C / MHz	241.43	289.36	236.37
D_J / kHz [b]	0.0182	0.0350	0.0113
D_{JK} / kHz	-0.0402	0.0000	-0.0051
D_K / kHz	0.1819	0.0216	0.1243
d_1 / kHz	-0.0039	0.0013	-0.0017
d_2 / kHz	-0.0001	-0.0009	-0.0001
$\lvert\mu_a\rvert$ / D	2.34	0.70	2.24
$\lvert\mu_b\rvert$ / D	1.01	1.36	1.33
$\lvert\mu_c\rvert$ / D	1.99	1.34	0.07
ΔE_{ZPE} / kJ mol^{-1} [c]	0.00	0.10	0.43
ΔG / kJ mol^{-1}	0.00	0.73	1.11
Ec / kJ mol^{-1}	-48.4	-50.6	-49.2

[a]Rotational constants (A, B, C). [b]Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2) and electric dipole moments (μ_α, α = a, b, c). [c]Relative energy with zero-point corrections (ΔE), Gibbs energy (ΔG, 298K, 1 atm) and complexation energy (ΔE_c including BSSE corrections).

Table S4. Prediction of the rotational and energetic parameters for 2-phenylethanol dimer using the MP2 method and a polarized triple-ζ basis set (def2-TZVP).

Isomer	(PhEthOH)2_01	(PhEthOH)2_02	(PhEthOH)2_03
	Ggπ+Ggπ-Lp-	Ggπ+Ggπ-Lp+	Ggπ-Ggπ-Lp-
A / MHz [a]	736.53	574.68	743.24
B / MHz	284.82	328.00	280.32
C / MHz	247.57	300.83	242.10
D_J / kHz [b]	0.0145	0.0291	0.0097
D_{JK} / kHz	-0.0243	0.0034	-0.0012
D_K / kHz	0.1317	0.0079	0.0983
d_1 / kHz	-0.0029	0.0004	-0.0015
d_2 / kHz	0.00	-0.0008	-0.0001
$\lvert\mu_a\rvert$ / D	2.38	0.78	2.28
$\lvert\mu_b\rvert$ / D	0.97	1.35	1.34
$\lvert\mu_c\rvert$ / D	2.06	1.39	0.08
ΔE_{ZPE} / kJ mol^{-1} [c]	0.00	0.74	0.27
ΔG / kJ mol^{-1}	0.00	0.66	0.62
Ec / kJ mol^{-1}	-50.8	-52.5	-51.6

[a]Rotational constants (A, B, C). [b]Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2) and electric dipole moments (μ_α, α = a, b, c). [c]Relative energy with zero-point corrections (ΔE), Gibbs energy (ΔG, 298K, 1 atm) and complexation energy (ΔE_c including BSSE corrections).

Table S5. Observed rotational transitions of isomer I (Ggπ+Ggπ-Lp-) of 2-phenylethanol dimer (Freq.), together with the differences with the calculated transitions (o.-c.) for the fit of Table 1 and estimated frequency uncertainties (unc.). All values in MHz.

N	*J'*	K_{-1}'	K_{+1}'	*J"*	$K_{-1}"$	$K_{+1}"$	*Freq.* / MHz	*o-c* / MHz	*unc.* / MHz
1	4	0	4	3	0	3	2031.7642	0.000	0.020
2	4	2	3	3	2	2	2054.2087	0.011	0.020
3	7	3	5	7	2	5	2056.7761	0.009	0.020
4	7	3	4	7	2	5	2077.3749	0.026	0.020
5	4	2	2	3	2	1	2078.5728	0.002	0.020
6	8	2	7	8	1	8	2082.3365	-0.011	0.020
7	3	1	2	2	0	2	2110.3993	-0.007	0.020
8	4	1	3	3	1	2	2128.4044	0.004	0.020
9	6	3	4	6	2	4	2137.2355	0.008	0.020
10	5	3	3	5	2	3	2192.7230	0.002	0.020
11	4	3	2	4	2	2	2226.6654	-0.004	0.020
12	5	0	5	4	1	4	2235.3552	-0.001	0.020
13	4	3	1	4	2	3	2264.1694	0.002	0.020
14	5	3	2	5	2	4	2279.3915	0.000	0.020
15	6	3	4	6	2	5	2298.8823	0.002	0.020
16	6	3	3	6	2	5	2307.2145	-0.006	0.020
17	4	1	4	3	0	3	2319.4854	0.006	0.020
18	7	3	4	7	2	6	2353.6753	-0.008	0.020
19	2	2	0	1	1	0	2364.3431	-0.016	0.020
20	8	3	6	8	2	7	2381.8988	0.000	0.020
21	2	2	1	1	1	1	2400.6424	-0.004	0.020
22	8	3	5	8	2	7	2426.3277	0.046	0.020
23	5	1	5	4	1	4	2463.2804	-0.011	0.020
24	5	0	5	4	0	4	2523.0783	0.007	0.020
25	7	1	6	6	2	4	2564.0133	-0.012	0.020
26	5	2	4	4	2	3	2564.6254	0.000	0.020
27	5	4	2	4	4	1	2575.7364	0.009	0.020
28	5	4	1	4	4	0	2575.7364	-0.018	0.020
29	5	3	3	4	3	2	2577.7462	-0.005	0.020
30	5	3	2	4	3	1	2579.8490	-0.001	0.020
31	5	2	3	4	2	2	2611.6983	-0.001	0.020
32	5	1	4	4	1	3	2655.1195	0.006	0.020
33	11	2	10	11	1	11	2681.5347	0.025	0.020
34	4	1	3	3	0	3	2706.6238	0.002	0.020
35	5	1	5	4	0	4	2751.0049	-0.001	0.020
36	6	0	6	5	1	5	2778.3546	-0.007	0.020
37	9	2	7	8	3	5	2783.5375	0.008	0.020
38	12	4	9	12	3	9	2793.7216	0.014	0.020
39	3	2	2	2	1	1	2837.1182	0.006	0.020
40	3	2	1	2	1	1	2849.5326	0.000	0.020
41	11	2	10	10	3	7	2887.3423	0.008	0.020
42	11	3	8	11	2	10	2891.3394	0.011	0.020
43	11	4	8	11	3	8	2910.4835	0.001	0.020
44	6	1	6	5	1	5	2950.5197	0.007	0.020
45	3	2	2	2	1	2	2953.4718	0.005	0.020
46	3	2	1	2	1	2	2965.8769	-0.011	0.020
47	10	4	7	10	3	7	2997.7744	0.005	0.020
48	6	0	6	5	0	5	3006.3025	0.006	0.020

49	10	4	6	10	3	7	3007.5315	0.004	0.020
50	12	3	10	11	4	8	3024.7118	0.000	0.020
51	9	4	6	9	3	6	3059.1943	0.005	0.020
52	6	2	5	5	2	4	3072.9981	0.002	0.020
53	8	1	7	7	2	5	3075.2559	-0.006	0.020
54	6	5	2	5	5	1	3090.4736	0.004	0.020
55	6	5	1	5	5	0	3090.4736	0.003	0.020
56	6	4	3	5	4	2	3092.6757	0.012	0.020
57	6	4	2	5	4	1	3092.7649	-0.020	0.020
58	6	3	4	5	3	3	3095.2894	0.002	0.020
59	8	4	5	8	3	5	3099.8782	0.006	0.020
60	6	3	3	5	3	2	3100.8254	0.000	0.020
61	7	4	4	7	3	4	3125.2413	-0.009	0.020
62	7	4	3	7	3	4	3125.8073	0.006	0.020
63	6	4	3	6	3	3	3140.1286	-0.008	0.020
64	8	4	5	8	3	6	3144.2595	0.004	0.020
65	9	4	6	9	3	7	3145.4024	0.010	0.020
66	8	4	4	8	3	6	3145.8893	-0.011	0.020
67	7	4	3	7	3	5	3146.3906	0.008	0.020
68	6	4	2	6	3	4	3148.6311	0.003	0.020
69	9	4	5	9	3	7	3149.6318	0.003	0.020
70	6	2	4	5	2	3	3150.7857	0.005	0.020
71	10	4	6	10	3	8	3161.1522	-0.003	0.020
72	6	1	5	5	1	4	3177.6826	0.006	0.020
73	6	1	6	5	0	5	3178.4478	0.000	0.020
74	11	4	7	11	3	9	3185.3758	0.000	0.020
75	12	4	8	12	3	10	3228.6176	-0.008	0.020
76	7	0	7	6	1	6	3311.0015	0.008	0.020
77	4	2	2	3	1	2	3329.4301	-0.003	0.020
78	5	1	4	4	0	4	3329.9788	0.008	0.020
79	8	1	7	7	2	6	3351.5959	0.000	0.020
80	14	4	10	14	3	12	3404.7260	-0.013	0.020
81	10	2	8	9	3	6	3408.8547	0.002	0.020
82	7	1	7	6	1	6	3435.5146	0.002	0.020
83	7	0	7	6	0	6	3483.1487	0.003	0.020
84	4	2	3	3	1	3	3525.2519	0.004	0.020
85	9	1	8	8	2	6	3544.7147	-0.006	0.020
86	15	1	14	15	0	15	3560.0620	0.008	0.020
87	7	2	6	6	2	5	3578.9471	0.005	0.020
88	7	6	1	6	6	0	3605.2619	0.006	0.020
89	7	6	2	6	6	1	3605.2619	0.006	0.020
90	7	5	3	6	5	2	3607.1280	0.006	0.020
91	7	5	2	6	5	1	3607.1280	0.000	0.020
92	7	1	7	6	0	6	3607.6621	-0.003	0.020
93	7	4	4	6	4	3	3610.5179	0.000	0.020
94	7	4	3	6	4	2	3610.9121	-0.006	0.020
95	7	3	5	6	3	4	3613.1705	0.007	0.020
96	7	3	4	6	3	3	3625.4038	-0.001	0.020
97	7	2	5	6	2	4	3693.6257	0.002	0.020
98	7	1	6	6	1	5	3694.7538	0.004	0.020
99	5	2	4	4	1	3	3728.8640	-0.001	0.020
100	15	5	11	15	4	11	3780.6456	-0.003	0.020
101	3	3	0	2	2	0	3796.5261	0.005	0.020
102	3	3	1	2	2	1	3798.9156	-0.003	0.020
103	5	2	3	4	1	3	3812.7367	0.004	0.020
104	8	0	8	7	1	7	3831.6223	0.009	0.020

105	14	5	10	14	4	10	3865.4325	0.019	0.020
106	8	1	8	7	1	7	3918.4181	-0.003	0.020
107	13	5	9	13	4	9	3926.5737	-0.008	0.020
108	8	0	8	7	0	7	3956.1302	-0.002	0.020
109	10	1	9	9	2	7	3965.4250	-0.010	0.020
110	9	1	8	8	2	7	3976.0625	-0.018	0.020
111	15	4	11	14	5	9	3983.1624	-0.008	0.020
112	6	1	5	5	0	5	3984.5751	-0.002	0.020
113	11	5	7	11	4	7	3999.3077	0.006	0.020
114	14	5	9	14	4	11	4001.3219	0.003	0.020
115	13	5	8	13	4	10	4004.3380	-0.002	0.020
116	15	5	10	15	4	12	4006.3321	0.001	0.020
117	12	5	7	12	4	9	4011.6553	-0.003	0.020
118	10	5	6	10	4	6	4019.5160	-0.014	0.020
119	10	5	5	10	4	6	4019.8398	0.008	0.020
120	11	5	7	11	4	8	4019.8398	-0.007	0.020
121	11	5	6	11	4	8	4020.6421	-0.003	0.020
122	11	2	9	10	3	7	4023.2625	0.002	0.020
123	9	5	5	9	4	5	4033.1526	-0.011	0.020
124	9	5	4	9	4	6	4037.5117	0.010	0.020
125	8	1	8	7	0	7	4042.9511	0.010	0.020
126	8	2	7	7	2	6	4082.1451	0.006	0.020
127	5	2	4	4	1	4	4116.0090	0.001	0.020
128	8	7	1	7	7	0	4120.0648	-0.004	0.020
129	8	7	2	7	7	1	4120.0648	-0.004	0.020
130	8	6	3	7	6	2	4121.7108	-0.003	0.020
131	8	6	2	7	6	1	4121.7108	-0.003	0.020
132	8	5	4	7	5	3	4124.5114	0.011	0.020
133	8	5	3	7	5	2	4124.5114	-0.011	0.020
134	8	4	5	7	4	4	4129.3635	0.002	0.020
135	8	4	4	7	4	3	4130.4570	0.003	0.020
136	8	3	6	7	3	5	4130.9369	0.000	0.020
137	6	2	5	5	1	4	4146.7571	0.009	0.020
138	8	3	5	7	3	4	4154.7366	-0.002	0.020
139	8	1	7	7	1	6	4204.8559	-0.004	0.020
140	8	2	6	7	2	5	4237.1699	0.005	0.020
141	15	3	13	14	4	10	4300.8911	0.024	0.020
142	4	3	2	3	2	1	4305.2300	-0.010	0.020
143	4	3	1	3	2	1	4305.9420	-0.002	0.020
144	6	2	4	5	1	4	4308.4047	0.004	0.020
145	4	3	2	3	2	2	4317.6620	0.001	0.020
146	11	1	10	10	2	8	4332.8478	0.005	0.020
147	9	0	9	8	1	8	4340.7445	-0.005	0.020
148	9	1	9	8	1	8	4399.4827	0.007	0.020
149	9	0	9	8	0	8	4427.5647	0.007	0.020
150	9	1	9	8	0	8	4486.2778	-0.007	0.020
151	9	2	8	8	2	7	4582.3377	0.005	0.020
152	12	2	10	11	3	8	4613.4140	-0.010	0.020
153	9	7	2	8	7	1	4636.3848	-0.010	0.020
154	9	7	3	8	7	2	4636.3848	-0.010	0.020
155	9	6	4	8	6	3	4638.7405	-0.001	0.020
156	9	6	3	8	6	2	4638.7405	-0.002	0.020
157	9	5	5	8	5	4	4642.7428	0.040	0.020
158	9	5	4	8	5	3	4642.7428	-0.032	0.020
159	9	3	7	8	3	6	4648.0618	0.002	0.020
160	9	4	6	8	4	5	4649.2018	0.006	0.020

161	9	4	5	8	4	4	4651.7878	0.000	0.020
162	7	1	6	6	0	6	4673.0206	-0.010	0.020
163	9	3	6	8	3	5	4689.8815	0.003	0.020
164	9	1	8	8	1	7	4706.6244	0.000	0.020
165	6	2	5	5	1	5	4725.7183	0.005	0.020
166	9	2	7	8	2	6	4778.4492	-0.003	0.020
167	5	3	3	4	2	2	4804.4144	-0.006	0.020
168	5	3	2	4	2	2	4807.2268	0.004	0.020
169	7	2	5	6	1	5	4824.3496	0.001	0.020
170	10	0	10	9	1	9	4840.1865	-0.003	0.020
171	5	3	3	4	2	3	4841.2165	0.002	0.020
172	5	3	2	4	2	3	4844.0409	0.024	0.020
173	15	6	10	15	5	10	4867.6016	-0.004	0.020
174	10	1	10	9	1	9	4878.9815	0.006	0.020
175	15	6	9	15	5	11	4885.7654	0.008	0.020
176	10	0	10	9	0	9	4898.9223	0.007	0.020
177	13	6	8	13	5	8	4909.8961	-0.003	0.020
178	10	1	10	9	0	9	4937.6947	-0.008	0.020
179	8	6	3	8	5	3	4951.0414	0.010	0.020
180	8	6	2	8	5	3	4951.0414	0.010	0.020
181	8	6	3	8	5	4	4951.0414	-0.019	0.020
182	8	6	2	8	5	4	4951.0414	-0.019	0.020
183	7	6	2	7	5	2	4953.8553	0.015	0.020
184	7	6	1	7	5	2	4953.8553	0.015	0.020
185	7	6	2	7	5	3	4953.8553	0.008	0.020
186	7	6	1	7	5	3	4953.8553	0.008	0.020
187	10	2	9	9	2	8	5079.3586	0.001	0.020
188	14	1	13	13	2	11	5118.8428	-0.015	0.020
189	10	9	1	9	9	0	5149.7461	0.010	0.020
190	10	9	2	9	9	1	5149.7461	0.010	0.020
191	10	8	2	9	8	1	5151.1122	-0.016	0.020
192	10	8	3	9	8	2	5151.1122	-0.016	0.020
193	10	7	3	9	7	2	5153.1776	-0.010	0.020
194	10	7	4	9	7	3	5153.1776	-0.010	0.020
195	10	6	5	9	6	4	5156.4200	0.007	0.020
196	10	6	4	9	6	3	5156.4200	0.003	0.020
197	10	5	6	9	5	5	5161.8251	0.003	0.020
198	10	5	5	9	5	4	5162.0148	-0.008	0.020
199	10	3	8	9	3	7	5163.9368	0.007	0.020
200	13	2	11	12	3	9	5166.6733	0.018	0.020
201	10	4	7	9	4	6	5169.9325	-0.002	0.020
202	10	4	6	9	4	5	5175.4547	-0.001	0.020
203	11	1	10	10	2	9	5196.1640	-0.001	0.020
204	10	1	9	9	1	8	5199.1673	0.001	0.020
205	4	4	1	3	3	0	5213.9321	0.058	0.020
206	4	4	0	3	3	0	5213.9321	0.054	0.020
207	4	4	1	3	3	1	5213.9321	-0.043	0.020
208	4	4	0	3	3	1	5213.9321	-0.047	0.020
209	10	3	7	9	3	6	5231.3539	-0.001	0.020
210	6	3	3	5	2	3	5296.3353	-0.014	0.020
211	9	2	8	8	1	7	5312.8774	0.001	0.020
212	10	2	8	9	2	7	5315.2069	0.005	0.020
213	11	0	11	10	1	10	5332.1219	0.018	0.020
214	7	2	6	6	1	6	5354.1510	0.008	0.020
215	11	1	11	10	1	10	5357.2339	-0.003	0.020
216	8	2	6	7	1	6	5366.7590	-0.004	0.020

217	11	0	11	10	0	10	5370.8972	0.006	0.020
218	6	3	4	5	2	4	5371.8790	0.002	0.020
219	6	3	3	5	2	4	5380.2364	0.019	0.020
220	15	3	12	14	4	10	5381.0566	0.006	0.020
221	8	1	7	7	0	7	5394.7422	-0.003	0.020
222	11	1	11	10	0	10	5396.0353	0.012	0.020
223	11	2	10	10	2	9	5573.1560	-0.003	0.020
224	11	9	2	10	9	1	5665.9026	0.008	0.020
225	11	9	3	10	9	2	5665.9026	0.008	0.020
226	11	8	3	10	8	2	5667.7419	-0.011	0.020
227	11	8	4	10	8	3	5667.7419	-0.011	0.020
228	11	7	5	10	7	4	5670.5047	0.006	0.020
229	11	7	4	10	7	3	5670.5047	0.005	0.020
230	14	2	12	13	3	10	5672.1167	-0.001	0.020
231	11	6	6	10	6	5	5674.7922	-0.010	0.020
232	11	6	5	10	6	4	5674.7922	-0.022	0.020
233	11	3	9	10	3	8	5677.9361	-0.007	0.020
234	11	5	7	10	5	6	5681.9230	-0.013	0.020
235	11	1	10	10	1	9	5682.6232	0.014	0.020
236	11	4	8	10	4	7	5691.4204	0.044	0.020
237	11	4	7	10	4	6	5702.1950	0.031	0.020
238	7	3	4	6	2	4	5770.9641	-0.009	0.020
239	11	3	8	10	3	7	5778.6457	-0.017	0.020
240	12	0	12	11	1	11	5818.5157	0.000	0.020
241	12	1	12	11	1	11	5834.5591	0.007	0.020
242	12	7	6	12	6	6	5839.8674	0.023	0.020
243	12	7	5	12	6	6	5839.8674	0.022	0.020
244	12	0	12	11	0	11	5843.6492	0.001	0.020
245	11	7	5	11	6	5	5845.4755	-0.002	0.020
246	11	7	4	11	6	5	5845.4755	-0.002	0.020
247	11	7	5	11	6	6	5845.4755	-0.020	0.020
248	11	7	4	11	6	6	5845.4755	-0.020	0.020
249	11	2	9	10	2	8	5845.7777	0.015	0.020
250	9	7	2	9	6	3	5853.0329	0.010	0.020
251	9	7	3	9	6	3	5853.0329	0.010	0.020
252	9	7	2	9	6	4	5853.0329	0.009	0.020
253	9	7	3	9	6	4	5853.0329	0.009	0.020
254	12	1	12	11	0	11	5859.6816	-0.002	0.020
255	7	3	5	6	2	5	5912.0568	0.013	0.020
256	7	3	4	6	2	5	5932.5975	-0.028	0.020
257	9	2	7	8	1	7	5940.3741	0.019	0.020
258	8	2	7	7	1	7	6000.7671	-0.002	0.020
259	11	2	10	10	1	9	6059.6079	0.004	0.020
260	12	2	11	11	2	10	6063.8006	-0.001	0.020
261	9	1	8	8	0	8	6145.2264	-0.011	0.020
262	12	1	11	11	1	10	6158.3546	-0.002	0.020
263	12	11	1	11	11	0	6179.4246	-0.006	0.020
264	12	11	2	11	11	1	6179.4246	-0.006	0.020
265	12	10	2	11	10	1	6180.6764	-0.006	0.020
266	12	10	3	11	10	2	6180.6764	-0.006	0.020
267	12	9	3	11	9	2	6182.3890	-0.004	0.020
268	12	9	4	11	9	3	6182.3890	-0.004	0.020
269	12	8	4	11	8	3	6184.8140	0.003	0.020
270	12	8	5	11	8	4	6184.8140	0.003	0.020
271	8	3	6	7	2	5	6187.7064	0.002	0.020
272	12	7	6	11	7	5	6188.3837	-0.001	0.020

273	12	7	5	11	7	4	6188.3837	-0.001	0.020
274	12	3	10	11	3	9	6189.5409	-0.001	0.020
275	12	6	7	11	6	6	6194.0058	0.023	0.020
276	12	6	6	11	6	5	6194.0058	-0.012	0.020
277	12	5	8	11	5	7	6203.0945	-0.001	0.020
278	12	5	7	11	5	6	6204.2160	0.001	0.020
279	12	4	9	11	4	8	6213.1967	-0.005	0.020
280	8	3	5	7	2	5	6232.0857	-0.002	0.020
281	12	4	8	11	4	7	6232.7899	-0.003	0.020
282	6	4	3	5	3	2	6240.9603	-0.002	0.020
283	6	4	2	5	3	2	6241.1214	0.008	0.020
284	6	4	3	5	3	3	6243.7598	-0.005	0.020
285	6	4	2	5	3	3	6243.7598	-0.156	0.020
286	13	0	13	12	1	12	6301.0724	0.002	0.020
287	13	1	13	12	1	12	6311.1767	0.002	0.020
288	13	0	13	12	0	12	6317.1026	-0.004	0.020
289	13	0	13	12	0	12	6317.1026	-0.004	0.020
290	13	1	13	12	0	12	6327.2024	-0.008	0.020
291	12	3	9	11	3	8	6329.9713	-0.006	0.020
292	13	1	12	12	2	11	6346.3678	-0.009	0.020
293	12	2	10	11	2	9	6368.8265	0.000	0.020
294	8	3	6	7	2	6	6464.0453	0.007	0.020
295	8	3	5	7	2	6	6508.4325	0.011	0.020
296	10	2	8	9	1	8	6548.9282	-0.004	0.020
297	13	2	12	12	2	11	6551.4660	-0.002	0.020
298	9	3	7	8	2	6	6598.5962	-0.002	0.020
299	13	1	12	12	1	11	6628.8140	-0.002	0.020
300	5	5	1	4	4	0	6630.0720	0.004	0.020
301	5	5	0	4	4	0	6630.0720	0.004	0.020
302	5	5	1	4	4	1	6630.0720	0.001	0.020
303	5	5	0	4	4	1	6630.0720	0.001	0.020
304	9	2	8	8	1	8	6664.6882	0.007	0.020
305	9	3	6	8	2	6	6684.8010	0.000	0.020
306	13	11	2	12	11	1	6695.5023	0.017	0.020
307	13	11	3	12	11	2	6695.5023	0.017	0.020
308	13	10	3	12	10	2	6697.0774	-0.005	0.020
309	13	10	4	12	10	3	6697.0774	-0.005	0.020
310	13	3	11	12	3	10	6698.2479	0.000	0.020
311	13	9	4	12	9	3	6699.2730	0.011	0.020
312	13	9	5	12	9	4	6699.2730	0.011	0.020
313	13	8	5	12	8	4	6702.3394	-0.004	0.020
314	13	8	6	12	8	5	6702.3394	-0.004	0.020
315	13	7	7	12	7	6	6706.9013	0.003	0.020
316	13	7	6	12	7	5	6706.9013	0.001	0.020
317	13	6	8	12	6	7	6714.0738	0.046	0.020
318	13	6	7	12	6	6	6714.0738	-0.044	0.020
319	13	5	9	12	5	8	6725.3116	-0.001	0.020
320	13	5	8	12	5	7	6727.6504	-0.004	0.020
321	15	8	8	15	7	8	6731.0787	0.021	0.020
322	15	8	7	15	7	8	6731.0787	0.021	0.020
323	15	8	8	15	7	9	6731.0787	-0.003	0.020
324	15	8	7	15	7	9	6731.0787	-0.004	0.020
325	13	4	10	12	4	9	6734.9746	0.002	0.020
326	14	8	7	14	7	7	6738.1260	0.010	0.020
327	14	8	6	14	7	7	6738.1260	0.010	0.020
328	14	8	7	14	7	8	6738.1260	0.001	0.020

329	14	8	6	14	7	8	6738.1260	0.001	0.020
330	13	8	5	13	7	6	6743.8271	-0.001	0.020
331	13	8	6	13	7	6	6743.8271	-0.001	0.020
332	13	8	5	13	7	7	6743.8271	-0.004	0.020
333	13	8	6	13	7	7	6743.8271	-0.004	0.020
334	12	8	4	12	7	5	6748.3865	0.001	0.020
335	12	8	5	12	7	5	6748.3865	0.001	0.020
336	12	8	4	12	7	6	6748.3865	0.000	0.020
337	12	8	5	12	7	6	6748.3865	0.000	0.020
338	7	4	4	6	3	3	6750.6614	0.007	0.020
339	7	4	3	6	3	3	6751.1924	-0.014	0.020
340	11	8	3	11	7	4	6751.9603	0.001	0.020
341	11	8	4	11	7	4	6751.9603	0.001	0.020
342	11	8	3	11	7	5	6751.9603	0.001	0.020
343	11	8	4	11	7	5	6751.9603	0.001	0.020
344	10	8	2	10	7	3	6754.6929	-0.013	0.020
345	10	8	2	10	7	4	6754.6929	-0.013	0.020
346	10	8	3	10	7	3	6754.6929	-0.013	0.020
347	10	8	3	10	7	4	6754.6929	-0.013	0.020
348	10	8	3	10	7	4	6754.6929	-0.013	0.020
349	9	8	1	9	7	2	6756.7422	-0.022	0.020
350	9	8	1	9	7	3	6756.7422	-0.022	0.020
351	9	8	2	9	7	2	6756.7422	-0.022	0.020
352	9	8	2	9	7	3	6756.7422	-0.022	0.020
353	7	4	4	6	3	4	6758.9921	-0.003	0.020
354	7	4	3	6	3	4	6759.5476	0.001	0.020
355	13	4	9	12	4	8	6768.3299	-0.005	0.020
356	14	0	14	13	1	13	6781.0078	0.001	0.020
357	14	1	14	13	1	13	6787.3046	-0.002	0.020
358	14	0	14	13	0	13	6791.1110	0.000	0.020
359	14	1	14	13	0	13	6797.4191	0.008	0.020
360	13	3	10	12	3	9	6882.3878	-0.003	0.020
361	13	2	11	12	2	10	6883.2076	-0.001	0.020
362	14	1	13	13	2	12	6891.5546	0.006	0.020
363	10	1	9	9	0	9	6916.8452	0.000	0.020
364	10	3	8	9	2	7	6984.0610	-0.015	0.020
365	9	3	7	8	2	7	7029.9606	0.002	0.020
366	14	2	13	13	2	12	7036.4456	0.004	0.020
367	14	1	13	13	1	12	7096.6404	0.000	0.020
368	10	3	7	9	2	7	7137.7086	0.005	0.020
369	6	5	2	5	4	1	7144.7976	0.014	0.020
370	6	5	1	5	4	1	7144.7976	0.013	0.020
371	6	5	2	5	4	2	7144.7976	-0.016	0.020
372	6	5	1	5	4	2	7144.7976	-0.017	0.020
373	11	2	9	10	1	9	7195.5240	-0.005	0.020
374	14	3	12	13	3	11	7203.6813	-0.004	0.020
375	14	12	2	13	12	1	7210.2784	-0.021	0.020
376	14	12	3	13	12	2	7210.2784	-0.021	0.020
377	14	11	3	13	11	2	7211.8049	-0.001	0.020
378	14	11	4	13	11	3	7211.8049	-0.001	0.020
379	14	10	4	13	10	3	7213.8067	0.001	0.020
380	14	10	5	13	10	4	7213.8067	0.001	0.020
381	14	9	5	13	9	4	7216.5367	0.003	0.020
382	14	9	6	13	9	5	7216.5367	0.003	0.020
383	14	8	7	13	8	6	7220.3943	0.004	0.020
384	14	8	6	13	8	5	7220.3943	0.004	0.020

385	14	7	8	13	7	7	7226.0930	-0.004	0.020
386	14	7	7	13	7	6	7226.0930	-0.010	0.020
387	14	6	9	13	6	8	7235.0053	-0.003	0.020
388	14	6	8	13	6	7	7235.2088	-0.010	0.020
389	14	2	13	13	1	12	7241.5475	0.013	0.020
390	14	5	10	13	5	9	7248.5438	0.000	0.020
391	14	5	9	13	5	8	7253.1262	-0.005	0.020
392	8	4	5	7	3	4	7254.6030	-0.008	0.020
393	14	4	11	13	4	10	7256.1560	0.003	0.020
394	8	4	4	7	3	4	7256.2622	0.007	0.020
395	15	0	15	14	1	14	7259.2103	0.001	0.020
396	15	1	15	14	1	14	7263.0950	-0.008	0.020
397	15	0	15	14	0	14	7265.5108	0.002	0.020
398	15	1	15	14	0	14	7269.3970	-0.006	0.020
399	8	4	5	7	3	5	7275.1967	0.004	0.020
400	8	4	4	7	3	5	7276.8257	-0.011	0.020
401	14	4	10	13	4	9	7309.7102	-0.001	0.020
402	10	2	9	9	1	9	7344.5693	0.006	0.020
403	11	3	9	10	2	8	7346.8138	-0.004	0.020
404	14	2	12	13	2	11	7387.8580	0.005	0.020
405	15	1	14	14	2	13	7419.0647	-0.009	0.020
406	14	3	11	13	3	10	7432.6496	-0.004	0.020
407	15	2	14	14	2	13	7519.0726	-0.003	0.020
408	15	1	14	14	1	13	7563.9721	0.006	0.020
409	11	3	8	10	2	8	7601.1667	0.001	0.020
410	10	3	8	9	2	8	7611.5574	0.003	0.020
411	11	9	2	11	8	3	7656.2201	0.011	0.020
412	11	9	2	11	8	4	7656.2201	0.011	0.020
413	11	9	3	11	8	3	7656.2201	0.011	0.020
414	11	9	3	11	8	4	7656.2201	0.011	0.020
415	7	5	3	6	4	3	7659.2351	-0.037	0.020
416	7	5	2	6	4	3	7659.2351	-0.044	0.020
417	15	3	13	14	3	12	7705.6008	-0.006	0.020
418	15	11	4	14	11	3	7728.4245	0.013	0.020
419	15	11	5	14	11	4	7728.4245	0.013	0.020
420	15	10	5	14	10	4	7730.8727	-0.004	0.020
421	15	10	6	14	10	5	7730.8727	-0.004	0.020
422	15	9	6	14	9	5	7734.2464	0.007	0.020
423	15	9	7	14	9	6	7734.2464	0.007	0.020
424	15	8	8	14	8	7	7738.9901	-0.005	0.020
425	15	8	7	14	8	6	7738.9901	-0.006	0.020
426	15	7	9	14	7	8	7746.0394	0.002	0.020
427	15	7	8	14	7	7	7746.0394	-0.014	0.020
428	9	4	6	8	3	5	7749.0685	0.000	0.020
429	9	4	5	8	3	5	7753.3062	0.001	0.020
430	15	6	10	14	6	9	7756.9899	0.004	0.020
431	15	6	9	14	6	8	7757.4439	-0.004	0.020
432	15	5	11	14	5	10	7772.6574	-0.010	0.020
433	15	4	12	14	4	11	7776.1509	0.007	0.020
434	15	5	10	14	5	9	7781.1594	0.003	0.020
435	9	4	6	8	3	6	7793.4576	0.006	0.020
436	15	4	11	14	4	10	7857.4277	-0.004	0.020
437	15	2	13	14	2	12	7882.0949	0.002	0.020
438	15	3	12	14	3	11	7977.8984	0.002	0.020

Table S6. Observed rotational transitions of isomer II (Ggπ+Ggπ-Lp+) of 2-phenylethanol dimer (Freq.), together with the differences with the calculated transitions (o.-c.) for the fit of Table 1 and estimated frequency uncertainties (unc.). All values in MHz.

N	*J'*	K_{-1}'	K_{+1}'	*J"*	$K_{-1}"$	$K_{+1}"$	*Freq.* / MHz	*o-c* / MHz	*unc.* / MHz
1	4	0	4	3	1	3	2188.4971	0.005	0.020
2	4	1	4	3	0	3	2534.9139	-0.0045	0.020
3	3	2	1	2	1	2	2639.0969	-0.0028	0.020
4	4	1	3	3	0	3	2800.5235	-0.0085	0.020
5	5	0	5	4	1	4	2808.2339	0.0081	0.020
6	7	6	1	7	5	2	2887.3423	0.0142	0.020
7	7	6	2	7	5	2	2887.3423	0.0142	0.020
8	7	6	2	7	5	3	2887.3423	0.0054	0.020
9	7	6	1	7	5	3	2887.3423	0.0053	0.020
10	6	6	0	6	5	1	2888.8591	0.0098	0.020
11	6	6	1	6	5	1	2888.8591	0.0098	0.020
12	6	6	1	6	5	2	2888.8591	0.0083	0.020
13	6	6	0	6	5	2	2888.8591	0.0083	0.020
14	5	1	5	4	1	4	2925.4830	-0.0251	0.020
15	5	0	5	4	0	4	2962.6921	0.0051	0.020
16	6	1	5	5	2	3	2995.2486	-0.0006	0.020
17	5	2	4	4	2	3	2995.4900	0.0128	0.020
18	5	1	5	4	0	4	3079.9652	-0.0042	0.020
19	4	2	3	3	1	2	3108.9862	-0.0041	0.020
20	3	3	1	2	2	0	3114.4658	0.0158	0.020
21	3	3	1	2	2	1	3116.4686	0.0008	0.020
22	3	3	0	2	2	1	3116.5610	-0.0026	0.020
23	4	2	2	3	1	2	3138.5050	-0.0102	0.020
24	4	2	3	3	1	3	3268.6681	0.004	0.020
25	10	7	4	10	6	4	3408.4852	0.0113	0.020
26	10	7	3	10	6	4	3408.4852	0.0112	0.020
27	10	7	4	10	6	4	3408.4852	0.0113	0.020
28	10	7	3	10	6	4	3408.4852	0.0112	0.020
29	10	7	4	10	6	5	3408.4852	0.0032	0.020
30	10	7	3	10	6	5	3408.4852	0.0031	0.020
31	9	7	3	9	6	3	3411.1002	0.0006	0.020
32	9	7	2	9	6	3	3411.1002	0.0006	0.020
33	9	7	2	9	6	4	3411.1002	-0.0014	0.020
34	9	7	3	9	6	4	3411.1002	-0.0014	0.020
35	8	7	2	8	6	2	3413.0101	0.0022	0.020
36	8	7	1	8	6	2	3413.0101	0.0022	0.020
37	8	7	2	8	6	3	3413.0101	0.0018	0.020
38	8	7	1	8	6	3	3413.0101	0.0018	0.020
39	7	7	1	7	6	2	3414.3433	-0.0024	0.020
40	7	7	1	7	6	1	3414.3433	-0.0024	0.020
41	7	7	0	7	6	1	3414.3433	-0.0024	0.020
42	7	7	0	7	6	2	3414.3433	-0.0024	0.020
43	6	0	6	5	1	5	3422.0309	-0.0059	0.020
44	5	1	4	4	0	4	3476.7207	-0.0132	0.020
45	6	1	6	5	1	5	3506.3891	-0.0034	0.020
46	6	0	6	5	0	5	3539.3210	0.0017	0.020
47	6	2	5	5	2	4	3590.8890	-0.0072	0.020
48	7	1	6	6	2	4	3604.4500	0.018	0.020

49	6	3	4	5	3	3	3608.5480	0.0034	0.020
50	6	3	3	5	3	2	3613.8006	0.0263	0.020
51	6	1	6	5	0	5	3623.6720	-0.003	0.020
52	6	2	4	5	2	3	3651.3813	-0.0002	0.020
53	6	1	5	5	1	4	3660.9223	-0.0088	0.020
54	4	3	2	3	2	1	3710.2166	0.0087	0.020
55	4	3	1	3	2	1	3710.8794	0.0023	0.020
56	4	3	2	3	2	2	3720.2290	0.0082	0.020
57	4	3	1	3	2	2	3720.8927	0.0027	0.020
58	5	2	3	4	1	3	3722.3353	-0.0057	0.020
59	7	1	6	6	2	5	3731.6825	-0.0015	0.020
60	5	2	4	4	1	4	3921.1830	-0.0049	0.020
61	13	8	6	13	7	6	3928.0839	0.0162	0.020
62	13	8	5	13	7	6	3928.0839	0.0161	0.020
63	13	8	6	13	7	7	3928.0839	0.0107	0.020
64	13	8	5	13	7	7	3928.0839	0.0106	0.020
65	12	8	5	12	7	5	3931.7673	-0.0092	0.020
66	12	8	4	12	7	5	3931.7673	-0.0093	0.020
67	12	8	5	12	7	6	3931.7673	-0.0109	0.020
68	12	8	4	12	7	6	3931.7673	-0.0109	0.020
69	11	8	4	11	7	4	3934.6752	-0.0088	0.020
70	11	8	3	11	7	4	3934.6752	-0.0088	0.020
71	11	8	4	11	7	5	3934.6752	-0.0092	0.020
72	11	8	3	11	7	5	3934.6752	-0.0092	0.020
73	5	2	3	4	1	4	3987.9430	-0.0116	0.020
74	7	0	7	6	1	6	4027.7499	-0.0121	0.020
75	7	1	7	6	1	6	4085.6591	0.0093	0.020
76	7	1	7	6	0	6	4169.9985	-0.007	0.020
77	10	3	8	9	4	5	4174.9646	0.0746	0.020
78	6	1	5	5	0	5	4174.9646	-0.0135	0.020
79	6	2	5	5	1	4	4189.8229	0.0113	0.020
80	4	4	1	3	3	0	4241.5900	-0.0155	0.020
81	4	4	0	3	3	0	4241.5900	-0.0193	0.020
82	4	4	1	3	3	1	4241.6975	-0.0039	0.020
83	4	4	0	3	3	1	4241.6975	-0.0077	0.020
84	7	1	6	6	1	5	4260.5570	-0.0073	0.020
85	7	2	5	6	2	4	4271.7251	0.0007	0.020
86	5	3	3	4	2	2	4298.2416	0.0047	0.020
87	5	3	2	4	2	2	4300.8901	-0.006	0.020
88	6	2	4	5	1	4	4317.0553	-0.0081	0.020
89	10	3	7	9	4	6	4318.9528	0.0196	0.020
90	5	3	3	4	2	3	4327.7680	0.0063	0.020
91	5	3	2	4	2	3	4330.4074	-0.0136	0.020
92	8	1	7	7	2	6	4401.6852	-0.004	0.020
93	15	9	7	15	8	7	4451.1285	0.0102	0.020
94	15	9	6	15	8	7	4451.1285	0.0102	0.020
95	15	9	7	15	8	8	4451.1285	0.0091	0.020
96	15	9	6	15	8	8	4451.1285	0.0091	0.020
97	14	9	6	14	8	6	4454.9913	-0.0006	0.020
98	14	9	5	14	8	6	4454.9913	-0.0006	0.020
99	14	9	6	14	8	7	4454.9913	-0.001	0.020
100	14	9	5	14	8	7	4454.9913	-0.001	0.020
101	13	9	5	13	8	5	4458.1240	-0.0087	0.020
102	13	9	4	13	8	5	4458.1240	-0.0087	0.020
103	13	9	5	13	8	6	4458.1240	-0.0087	0.020
104	13	9	4	13	8	6	4458.1240	-0.0087	0.020

105	12	9	4	12	8	5	4460.6266	-0.0155	0.020
106	12	9	4	12	8	4	4460.6266	-0.0154	0.020
107	12	9	3	12	8	5	4460.6266	-0.0155	0.020
108	12	9	3	12	8	4	4460.6266	-0.0154	0.020
109	11	9	3	11	8	4	4462.6152	0.0026	0.020
110	11	9	3	11	8	3	4462.6152	0.0026	0.020
111	11	9	2	11	8	4	4462.6152	0.0026	0.020
112	11	9	2	11	8	3	4462.6152	0.0026	0.020
113	10	9	2	10	8	3	4464.1358	0.0072	0.020
114	10	9	2	10	8	2	4464.1358	0.0072	0.020
115	10	9	1	10	8	3	4464.1358	0.0072	0.020
116	10	9	1	10	8	2	4464.1358	0.0072	0.020
117	6	2	5	5	1	5	4586.5591	-0.0169	0.020
118	8	0	8	7	1	7	4625.2131	0.0069	0.020
119	8	0	8	7	0	7	4683.0809	-0.013	0.020
120	7	2	6	6	1	5	4713.2487	-0.0064	0.020
121	8	1	8	7	0	7	4721.3239	-0.0001	0.020
122	8	2	7	7	2	6	4775.7032	0.0251	0.020
123	6	3	4	5	2	3	4874.0494	-0.0131	0.020
124	6	3	3	5	2	3	4881.9463	-0.0052	0.020
125	7	2	5	6	1	5	4927.8632	0.0065	0.020
126	6	3	4	5	2	4	4940.8060	-0.0231	0.020
127	6	3	3	5	2	4	4948.6887	-0.0294	0.020
128	15	10	6	15	9	7	4981.4773	-0.0017	0.020
129	15	10	6	15	9	6	4981.4773	-0.0017	0.020
130	15	10	5	15	9	7	4981.4773	-0.0017	0.020
131	15	10	5	15	9	6	4981.4773	-0.0017	0.020
132	9	0	9	8	1	8	5215.4840	0.0004	0.020
133	8	2	7	7	1	6	5228.3896	0.0206	0.020
134	9	1	9	8	1	8	5239.9621	-0.0181	0.020
135	9	0	9	8	0	8	5253.7000	-0.0136	0.020
136	7	2	6	6	1	6	5264.5680	0.0097	0.020
137	9	1	9	8	0	8	5278.2090	-0.0013	0.020
138	5	5	1	4	4	0	5367.7583	0.0009	0.020
139	5	5	0	4	4	0	5367.7583	0.0008	0.020
140	5	5	1	4	4	1	5367.7583	-0.0028	0.020
141	5	5	0	4	4	1	5367.7583	-0.0029	0.020
142	6	4	3	5	3	2	5440.5779	0.0162	0.020
143	6	4	2	5	3	2	5440.7403	0.0095	0.020
144	6	4	3	5	3	3	5443.2304	0.0093	0.020
145	6	4	2	5	3	3	5443.3745	-0.0155	0.020
146	8	2	6	7	1	6	5558.5664	0.0235	0.020
147	7	3	5	6	2	5	5561.1743	-0.0035	0.020
148	10	0	10	9	1	9	5800.2023	-0.0023	0.020
149	8	3	5	7	2	5	6017.2546	0.0012	0.020
150	7	4	4	6	3	3	6036.5731	-0.0038	0.020
151	7	4	3	6	3	3	6037.1995	0.0063	0.020
152	7	4	4	6	3	4	6044.4751	0.0089	0.020
153	7	4	3	6	3	4	6045.0775	-0.0047	0.020
154	10	2	8	9	2	7	6120.2334	0.0229	0.020
155	8	3	6	7	2	6	6190.4419	0.0051	0.020
156	9	2	7	8	1	7	6212.0530	-0.0095	0.020
157	8	3	5	7	2	6	6231.8515	-0.0033	0.020
158	10	2	9	9	1	8	6248.3703	0.0206	0.020
159	11	0	11	10	1	10	6380.9199	-0.0071	0.020
160	11	1	11	10	0	10	6405.6777	0.0022	0.020

161	6	6	1	5	5	0	6493.8501	0.0024	0.020
162	6	6	0	5	5	0	6493.8501	0.0024	0.020
163	6	6	1	5	5	1	6493.8501	0.0023	0.020
164	6	6	0	5	5	1	6493.8501	0.0023	0.020
165	7	5	3	6	4	2	6568.4837	-0.0001	0.020
166	7	5	2	6	4	2	6568.4837	-0.0089	0.020
167	7	5	3	6	4	3	6568.6439	-0.0089	0.020
168	7	5	2	6	4	3	6568.6439	-0.0177	0.020
169	9	3	6	8	2	6	6579.3047	0.0053	0.020
170	8	4	5	7	3	4	6627.4201	-0.0014	0.020
171	8	4	4	7	3	4	6629.2667	0.0133	0.020
172	8	4	5	7	3	5	6646.7892	0.0026	0.020
173	10	2	8	9	1	8	6890.7849	-0.0104	0.020
174	12	0	12	11	1	11	6958.9110	-0.0058	0.020
175	12	1	12	11	0	11	6974.0246	-0.0093	0.020
176	7	6	2	6	5	1	7094.4291	0.0006	0.020
177	7	6	1	6	5	1	7094.4291	0.0006	0.020
178	7	6	2	6	5	2	7094.4291	-0.0007	0.020
179	7	6	1	6	5	2	7094.4291	-0.0008	0.020
180	9	4	6	8	3	5	7209.7864	0.0088	0.020
181	9	4	5	8	3	5	7214.4872	0.0079	0.020
182	9	4	6	8	3	6	7251.2008	0.005	0.020
183	9	4	5	8	3	6	7255.8901	-0.0072	0.020
184	13	0	13	12	1	12	7535.0878	-0.0193	0.020
185	7	7	1	6	6	1	7619.9319	0.007	0.020
186	7	7	1	6	6	0	7619.9319	0.007	0.020
187	7	7	0	6	6	1	7619.9319	0.007	0.020
188	7	7	0	6	6	0	7619.9319	0.007	0.020
189	8	6	3	7	5	2	7694.8502	0.0084	0.020
190	8	6	2	7	5	2	7694.8502	0.008	0.020
191	8	6	3	7	5	3	7694.8502	-0.0004	0.020
192	8	6	2	7	5	3	7694.8502	-0.0008	0.020
193	11	3	8	10	2	8	7727.4017	0.0131	0.020

Table S7. Observed rotational transitions of isomer III (Ggπ-Ggπ-Lp-) of 2-phenylethanol dimer (Freq.), together with the differences with the calculated transitions (o.-c.) for the fit of Table 1 and estimated frequency uncertainties (unc.). All values in MHz.

N	*J'*	K_{-1}'	K_{+1}'	*J"*	$K_{-1}"$	$K_{+1}"$	*Freq.* / MHz	*o-c* / MHz	*unc.* / MHz
1	4	2	3	3	2	2	2018.6258	0.004	0.020
2	4	3	2	3	3	1	2025.0296	-0.016	0.020
3	4	3	1	3	3	0	2025.6107	-0.001	0.020
4	4	2	2	3	2	1	2042.1599	-0.005	0.020
5	4	1	3	3	1	2	2092.3765	-0.004	0.020
6	7	3	4	7	2	5	2130.1272	0.008	0.020
7	5	0	5	4	1	4	2182.2857	0.013	0.020
8	6	3	3	6	2	4	2197.1225	0.017	0.020
9	5	3	2	5	2	3	2245.8077	-0.002	0.020
10	4	3	1	4	2	2	2276.7029	-0.005	0.020
11	4	1	4	3	0	3	2294.7191	-0.001	0.020
12	4	3	2	4	2	3	2311.5676	-0.009	0.020
13	6	3	4	6	2	5	2345.8448	0.010	0.020
14	2	2	1	1	1	0	2373.2200	0.001	0.020
15	2	2	0	1	1	1	2414.1229	-0.004	0.020
16	5	1	5	4	1	4	2419.7717	-0.005	0.020
17	5	0	5	4	0	4	2480.0363	-0.005	0.020
18	10	2	9	10	1	10	2486.5613	-0.012	0.020
19	9	3	7	9	2	8	2490.2456	-0.006	0.020
20	5	2	4	4	2	3	2520.2709	0.004	0.020
21	5	4	2	4	4	1	2530.9688	-0.004	0.020
22	5	4	1	4	4	0	2530.9688	-0.029	0.020
23	5	3	3	4	3	2	2532.9540	0.001	0.020
24	5	3	2	4	3	1	2534.9148	-0.007	0.020
25	5	2	3	4	2	2	2565.8154	-0.004	0.020
26	10	3	8	10	2	9	2572.6288	0.005	0.020
27	5	1	4	4	1	3	2610.2997	0.000	0.020
28	5	1	5	4	0	4	2717.5378	-0.008	0.020
29	6	0	6	5	1	5	2717.6531	0.001	0.020
30	3	2	2	2	1	1	2839.8483	0.004	0.020
31	6	1	6	5	1	5	2898.4515	-0.001	0.020
32	13	3	11	13	2	12	2941.7878	0.023	0.020
33	6	0	6	5	0	5	2955.1535	-0.003	0.020
34	3	2	1	2	1	2	2967.3181	-0.008	0.020
35	11	4	7	11	3	8	3008.0670	-0.004	0.020
36	6	2	5	5	2	4	3019.9249	-0.002	0.020
37	6	5	2	5	5	1	3036.7801	0.004	0.020
38	6	5	1	5	5	0	3036.7801	0.003	0.020
39	6	3	4	5	3	3	3041.4991	0.001	0.020
40	6	3	3	5	3	2	3046.6975	0.003	0.020
41	10	4	6	10	3	7	3081.8083	-0.007	0.020
42	6	2	4	5	2	3	3095.5655	0.166	0.020
43	6	1	5	5	1	4	3124.2400	-0.004	0.020
44	9	4	5	9	3	6	3135.3958	0.013	0.020
45	6	1	6	5	0	5	3135.9617	0.004	0.020
46	8	4	4	8	3	5	3171.7699	0.006	0.020
47	7	4	3	7	3	4	3194.9414	0.012	0.020
48	6	4	2	6	3	3	3208.7709	0.017	0.020

49	8	4	5	8	3	6	3211.9791	-0.007	0.020
50	9	4	6	9	3	7	3212.6890	-0.003	0.020
51	7	4	4	7	3	5	3213.7465	-0.004	0.020
52	5	4	1	5	3	2	3216.4296	-0.011	0.020
53	6	4	3	6	3	4	3216.4296	-0.012	0.020
54	10	4	7	10	3	8	3217.9207	0.000	0.020
55	5	4	2	5	3	3	3219.0390	-0.002	0.020
56	11	4	8	11	3	9	3230.1428	0.013	0.020
57	7	0	7	6	1	6	3243.0476	0.002	0.020
58	8	1	7	7	2	6	3250.4759	0.003	0.020
59	12	4	9	12	3	10	3252.0271	-0.004	0.020
60	4	2	3	3	1	2	3286.8899	-0.010	0.020
61	7	1	7	6	1	6	3374.9534	0.001	0.020
62	7	0	7	6	0	6	3423.8415	-0.004	0.020
63	7	2	6	6	2	5	3517.2454	0.001	0.020
64	7	6	1	6	6	0	3542.6147	-0.005	0.020
65	7	6	2	6	6	1	3542.6147	-0.005	0.020
66	7	5	3	6	5	2	3544.4266	0.001	0.020
67	7	5	2	6	5	1	3544.4266	-0.004	0.020
68	7	4	4	6	4	3	3547.7156	0.001	0.020
69	7	4	3	6	4	2	3548.0756	-0.004	0.020
70	7	3	5	6	3	4	3550.4003	-0.005	0.020
71	4	2	2	3	1	3	3553.3270	0.001	0.020
72	7	1	7	6	0	6	3555.7554	0.002	0.020
73	7	3	4	6	3	3	3561.9054	0.001	0.020
74	7	2	5	6	2	4	3628.8832	-0.008	0.020
75	7	1	6	6	1	5	3632.9295	-0.004	0.020
76	5	2	4	4	1	3	3714.7923	0.006	0.020
77	8	0	8	7	1	7	3756.6016	0.000	0.020
78	3	3	1	2	2	0	3818.1144	-0.003	0.020
79	3	3	0	2	2	1	3820.6202	-0.001	0.020
80	8	1	8	7	1	7	3849.3881	0.000	0.020
81	9	1	8	8	2	7	3867.5168	0.005	0.020
82	8	0	8	7	0	7	3888.5104	0.002	0.020
83	8	1	8	7	0	7	3981.2980	0.003	0.020
84	8	2	7	7	2	6	4011.9068	0.005	0.020
85	13	5	8	13	4	9	4024.2738	-0.007	0.020
86	8	7	1	7	7	0	4048.4861	-0.003	0.020
87	8	7	2	7	7	1	4048.4861	-0.003	0.020
88	8	6	3	7	6	2	4050.0751	-0.007	0.020
89	8	6	2	7	6	1	4050.0751	-0.008	0.020
90	8	5	4	7	5	3	4052.7844	0.007	0.020
91	8	5	3	7	5	2	4052.7844	-0.012	0.020
92	8	4	5	7	4	4	4057.4978	0.003	0.020
93	8	4	4	7	4	3	4058.4928	0.001	0.020
94	8	3	6	7	3	5	4059.2613	0.001	0.020
95	12	5	7	12	4	8	4062.7741	0.008	0.020
96	15	5	11	15	4	12	4075.1402	0.000	0.020
97	8	3	5	7	3	4	4081.6576	0.000	0.020
98	11	5	6	11	4	7	4089.8393	-0.008	0.020
99	12	5	8	12	4	9	4097.7987	0.002	0.020
100	11	5	7	11	4	8	4107.9148	-0.001	0.020
101	10	5	5	10	4	6	4108.6057	0.005	0.020
102	10	5	6	10	4	7	4117.2411	0.000	0.020
103	9	5	4	9	4	5	4121.4034	-0.009	0.020
104	8	1	7	7	1	6	4134.9472	-0.005	0.020

105	8	2	6	7	2	5	4163.3649	-0.006	0.020
106	5	2	3	4	1	4	4180.1967	0.003	0.020
107	9	0	9	8	1	8	4258.6374	-0.002	0.020
108	4	3	2	3	2	1	4318.2052	-0.008	0.020
109	9	1	9	8	1	8	4321.9821	0.001	0.020
110	4	3	1	3	2	2	4330.8592	0.001	0.020
111	9	0	9	8	0	8	4351.4257	-0.001	0.020
112	9	1	9	8	0	8	4414.7633	-0.004	0.020
113	10	1	9	9	2	8	4477.8338	0.001	0.020
114	9	2	8	8	2	7	4503.6421	-0.004	0.020
115	7	2	6	6	1	5	4517.4104	-0.003	0.020
116	9	8	1	8	8	0	4554.3668	-0.004	0.020
117	9	8	2	8	8	1	4554.3668	-0.004	0.020
118	9	7	2	8	7	1	4555.8175	-0.007	0.020
119	9	7	3	8	7	2	4555.8175	-0.007	0.020
120	9	6	4	8	6	3	4558.0902	-0.006	0.020
121	9	6	3	8	6	2	4558.0902	-0.007	0.020
122	9	5	5	8	5	4	4561.9907	0.065	0.020
123	9	5	4	8	5	3	4561.9907	0.001	0.020
124	9	3	7	8	3	6	4567.5401	-0.004	0.020
125	9	4	6	8	4	5	4568.2473	-0.004	0.020
126	9	4	5	8	4	4	4570.6191	0.003	0.020
127	9	3	6	8	3	5	4606.9960	0.000	0.020
128	9	1	8	8	1	7	4628.9418	0.001	0.020
129	9	2	7	8	2	6	4695.9385	-0.003	0.020
130	10	0	10	9	1	9	4750.7932	-0.009	0.020
131	10	1	10	9	1	9	4793.0199	0.005	0.020
132	5	3	3	4	2	2	4809.0007	-0.001	0.020
133	10	0	10	9	0	9	4814.1451	0.002	0.020
134	5	3	2	4	2	3	4847.1518	-0.007	0.020
135	8	2	7	7	1	6	4896.3900	0.009	0.020
136	10	2	9	9	2	8	4992.3046	-0.002	0.020
137	13	6	7	13	5	8	5018.4888	-0.007	0.020
138	13	6	8	13	5	9	5022.1762	0.021	0.020
139	12	6	6	12	5	7	5031.4825	0.027	0.020
140	12	6	7	12	5	8	5033.1110	0.000	0.020
141	10	9	1	9	9	0	5060.2504	-0.010	0.020
142	10	9	2	9	9	1	5060.2504	-0.010	0.020
143	10	8	2	9	8	1	5061.6189	0.003	0.020
144	10	8	3	9	8	2	5061.6189	0.003	0.020
145	10	7	4	9	7	3	5063.6178	0.006	0.020
146	10	7	3	9	7	2	5063.6178	0.006	0.020
147	10	6	5	9	6	4	5066.7158	-0.016	0.020
148	10	6	4	9	6	3	5066.7158	-0.020	0.020
149	10	5	6	9	5	5	5071.9747	0.013	0.020
150	10	5	5	9	5	4	5072.1296	-0.010	0.020
151	10	3	8	9	3	7	5074.6859	0.007	0.020
152	11	1	10	10	2	9	5075.5504	0.028	0.020
153	10	4	7	9	4	6	5079.9187	0.011	0.020
154	10	4	6	9	4	5	5084.9440	-0.007	0.020
155	10	1	9	9	1	8	5113.9752	0.008	0.020
156	10	3	7	9	3	6	5138.5258	0.006	0.020
157	10	2	8	9	2	7	5224.3148	0.000	0.020
158	11	0	11	10	1	10	5235.1956	-0.001	0.020
159	4	4	1	3	3	0	5245.9782	0.005	0.020
160	4	4	0	3	3	1	5246.0600	-0.010	0.020

161	11	1	11	10	1	10	5262.7966	0.003	0.020
162	9	2	8	8	1	7	5265.0697	-0.006	0.020
163	11	0	11	10	0	10	5277.4053	-0.004	0.020
164	6	3	4	5	2	3	5284.6804	0.000	0.020
165	11	1	11	10	0	10	5305.0106	0.005	0.020
166	6	3	3	5	2	4	5373.5886	0.002	0.020
167	11	2	10	10	2	9	5477.8154	0.000	0.020
168	11	10	1	10	10	0	5566.1577	0.003	0.020
169	11	10	2	10	10	1	5566.1577	0.003	0.020
170	11	9	2	10	9	1	5567.4488	0.012	0.020
171	11	9	3	10	9	2	5567.4488	0.012	0.020
172	11	8	3	10	8	2	5569.2292	-0.012	0.020
173	11	8	4	10	8	3	5569.2292	-0.012	0.020
174	11	7	5	10	7	4	5571.8917	-0.010	0.020
175	11	7	4	10	7	3	5571.8917	-0.010	0.020
176	11	6	6	10	6	5	5576.0552	-0.006	0.020
177	11	6	5	10	6	4	5576.0552	-0.017	0.020
178	11	3	9	10	3	8	5580.0839	0.004	0.020
179	11	5	7	10	5	6	5582.9581	-0.005	0.020
180	11	5	6	10	5	5	5583.4001	-0.003	0.020
181	11	1	10	10	1	9	5589.9987	0.002	0.020
182	11	4	8	10	4	7	5592.2926	0.004	0.020
183	11	4	7	10	4	6	5602.1556	-0.001	0.020
184	10	2	9	9	1	8	5628.4361	-0.005	0.020
185	12	1	11	11	2	10	5655.9100	0.000	0.020
186	11	3	8	10	3	7	5675.8942	-0.007	0.020
187	12	1	12	11	1	11	5731.5899	-0.016	0.020
188	12	0	12	11	0	11	5741.4451	0.007	0.020
189	11	2	9	10	2	8	5746.8316	-0.002	0.020
190	7	3	4	6	2	5	5915.5575	-0.006	0.020
191	12	2	11	11	2	10	5960.2021	-0.015	0.020
192	12	7	5	12	6	6	5966.5193	0.022	0.020
193	11	7	4	11	6	5	5971.9319	-0.005	0.020
194	11	7	5	11	6	6	5971.9319	-0.020	0.020
195	10	7	3	10	6	4	5976.1009	-0.007	0.020
196	10	7	4	10	6	5	5976.1009	-0.011	0.020
197	9	7	2	9	6	3	5979.2125	-0.019	0.020
198	9	7	3	9	6	4	5979.2125	-0.020	0.020
199	12	1	11	11	1	10	6058.2073	0.004	0.020
200	12	11	1	11	11	0	6072.0504	0.001	0.020
201	12	11	2	11	11	1	6072.0504	0.001	0.020
202	12	10	2	11	10	1	6073.2694	-0.006	0.020
203	12	10	3	11	10	2	6073.2694	-0.006	0.020
204	12	9	3	11	9	2	6074.9419	0.001	0.020
205	12	9	4	11	9	3	6074.9419	0.001	0.020
206	12	8	4	11	8	3	6077.2858	-0.001	0.020
207	12	8	5	11	8	4	6077.2858	-0.001	0.020
208	12	7	6	11	7	5	6080.7386	-0.007	0.020
209	12	7	5	11	7	4	6080.7386	-0.007	0.020
210	12	3	10	11	3	9	6083.1991	-0.001	0.020
211	12	6	7	11	6	6	6086.1661	0.011	0.020
212	12	6	6	11	6	5	6086.1661	-0.019	0.020
213	12	5	8	11	5	7	6094.9824	-0.001	0.020
214	12	5	7	11	5	6	6095.9766	-0.001	0.020
215	12	4	9	11	4	8	6105.0951	-0.007	0.020
216	12	4	8	11	4	7	6123.0606	0.002	0.020

217	8	3	6	7	2	5	6170.0385	-0.017	0.020
218	13	1	13	12	1	12	6199.6990	-0.004	0.020
219	13	0	13	12	0	12	6206.1758	0.000	0.020
220	13	1	12	12	2	11	6216.4791	-0.010	0.020
221	12	3	9	11	3	8	6217.5674	0.003	0.020
222	6	4	3	5	3	2	6255.2991	-0.012	0.020
223	6	4	2	5	3	3	6258.0805	0.003	0.020
224	12	2	10	11	2	9	6262.2015	0.000	0.020
225	12	2	11	11	1	10	6362.5208	0.010	0.020
226	13	2	12	12	2	11	6439.6753	0.004	0.020
227	8	3	5	7	2	6	6479.9719	-0.006	0.020
228	13	1	12	12	1	11	6520.7982	0.001	0.020
229	9	3	7	8	2	6	6574.2373	0.009	0.020
230	13	11	2	12	11	1	6579.1174	-0.009	0.020
231	13	11	3	12	11	2	6579.1174	-0.009	0.020
232	13	10	3	12	10	2	6580.6851	0.000	0.020
233	13	10	4	12	10	3	6580.6851	0.000	0.020
234	13	9	4	12	9	3	6582.8072	0.002	0.020
235	13	9	5	12	9	4	6582.8072	0.002	0.020
236	13	3	11	12	3	10	6583.5590	-0.004	0.020
237	13	8	6	12	8	5	6585.7900	-0.001	0.020
238	13	8	5	12	8	4	6585.7900	-0.001	0.020
239	13	7	7	12	7	6	6590.1953	-0.002	0.020
240	13	7	6	12	7	5	6590.1953	-0.004	0.020
241	13	6	8	12	6	7	6597.1293	0.043	0.020
242	13	6	7	12	6	6	6597.1293	-0.034	0.020
243	13	5	9	12	5	8	6608.0452	0.003	0.020
244	13	5	8	12	5	7	6610.1180	-0.005	0.020
245	13	4	10	12	4	9	6617.9389	-0.005	0.020
246	13	4	9	12	4	8	6648.6043	-0.004	0.020
247	14	0	14	13	1	13	6660.1797	-0.007	0.020
248	14	1	14	13	1	13	6667.2859	-0.003	0.020
249	14	0	14	13	0	13	6671.4760	-0.002	0.020
250	5	5	1	4	4	0	6672.6112	0.000	0.020
251	5	5	0	4	4	1	6672.6112	-0.003	0.020
252	14	1	14	13	0	13	6678.5659	-0.014	0.020
253	13	2	12	12	1	11	6743.9956	0.017	0.020
254	7	4	4	6	3	3	6756.3306	-0.001	0.020
255	14	1	13	13	2	12	6757.1797	0.000	0.020
256	13	3	10	12	3	9	6760.8335	0.000	0.020
257	7	4	3	6	3	4	6764.6547	-0.004	0.020
258	13	2	11	12	2	10	6769.2650	0.003	0.020
259	14	2	13	13	2	12	6916.4317	-0.003	0.020
260	10	3	8	9	2	7	6952.9702	0.005	0.020
261	14	1	13	13	1	12	6980.3666	0.005	0.020
262	9	3	6	8	2	7	7075.0725	0.001	0.020
263	14	3	12	13	3	11	7080.7918	0.002	0.020
264	14	11	3	13	11	2	7086.4629	0.003	0.020
265	14	11	4	13	11	3	7086.4629	0.003	0.020
266	14	10	4	13	10	3	7088.4137	0.005	0.020
267	14	10	5	13	10	4	7088.4137	0.005	0.020
268	14	8	6	13	8	5	7094.7999	0.005	0.020
269	14	8	7	13	8	6	7094.7999	0.005	0.020
270	14	7	8	13	7	7	7100.3083	-0.003	0.020
271	14	7	7	13	7	6	7100.3083	-0.008	0.020
272	14	6	9	13	6	8	7108.9250	0.003	0.020

273	14	6	8	13	6	7	7109.0962	-0.007	0.020
274	14	5	10	13	5	9	7122.1061	-0.002	0.020
275	14	5	9	13	5	8	7126.1874	-0.001	0.020
276	15	0	15	14	1	14	7130.0954	0.003	0.020
277	14	4	11	13	4	10	7130.3064	-0.004	0.020
278	15	1	15	14	1	14	7134.5212	0.002	0.020
279	14	2	13	13	1	12	7139.6275	0.012	0.020
280	15	1	15	14	0	14	7141.6282	0.007	0.020
281	6	5	2	5	4	1	7178.4005	0.011	0.020
282	6	5	1	5	4	2	7178.4005	-0.018	0.020
283	14	4	10	13	4	9	7179.7254	0.000	0.020
284	8	4	5	7	3	4	7251.9211	-0.001	0.020
285	14	2	12	13	2	11	7266.9622	-0.002	0.020
286	8	4	4	7	3	5	7272.7465	0.001	0.020
287	15	1	14	14	2	13	7279.8400	0.003	0.020
288	14	3	11	13	3	10	7302.5676	-0.001	0.020
289	11	3	9	10	2	8	7308.7336	0.003	0.020
290	15	2	14	14	2	13	7390.8370	0.000	0.020
291	15	1	14	14	1	13	7439.0922	0.000	0.020
292	15	3	13	14	3	12	7574.6123	-0.002	0.020
293	15	10	5	14	10	4	7596.4577	-0.013	0.020
294	15	9	6	14	9	5	7599.7380	0.004	0.020
295	15	9	7	14	9	6	7599.7380	0.004	0.020
296	15	8	8	14	8	7	7604.3441	0.006	0.020
297	15	8	7	14	8	6	7604.3441	0.006	0.020
298	15	7	9	14	7	8	7611.1549	0.012	0.020
299	15	7	8	14	7	7	7611.1549	-0.002	0.020
300	15	6	10	14	6	9	7621.7240	0.000	0.020
301	15	6	9	14	6	8	7622.1263	0.003	0.020
302	15	5	11	14	5	10	7637.0803	0.001	0.020
303	15	4	12	14	4	11	7641.6434	0.010	0.020
304	15	5	10	14	5	9	7644.6444	0.003	0.020
305	12	3	10	11	2	9	7645.1068	0.009	0.020
306	10	3	7	9	2	8	7709.9425	-0.002	0.020
307	15	4	11	14	4	10	7717.0135	0.001	0.020
308	9	4	6	8	3	5	7738.5040	-0.011	0.020
309	15	2	13	14	2	12	7754.5638	0.001	0.020
310	15	3	12	14	3	11	7839.8865	-0.004	0.020

Table S8. Equilibrium coordinates for isomer I (Ggπ+Ggπ-Lp-) of 2-phenylethanol dimer, according to the prediction with B3LYP-D3(BJ) /def2TZVP.

Atom	*a* / Å[a]	*b* / Å	*c* / Å
C	-2.7787	0.4672	1.2430
C	-2.3165	1.1881	0.1413
C	-2.6317	0.7224	-1.1348
C	-3.3939	-0.4274	-1.3069
C	-3.8525	-1.1326	-0.2013
C	-3.5399	-0.6819	1.0768
H	-2.5436	0.8150	2.2422
H	-2.2780	1.2695	-1.9997
H	-3.6318	-0.7702	-2.3058
H	-4.4508	-2.0248	-0.3330
H	-3.8957	-1.2231	1.9444
C	-1.4623	2.4141	0.3261
H	-1.7786	2.9580	1.2205
H	-1.5833	3.0863	-0.5256
C	0.0249	2.0873	0.4743
H	0.5915	3.0076	0.6205
H	0.1860	1.4438	1.3450
O	0.5666	1.4777	-0.6924
H	0.2499	0.5654	-0.7512
C	1.9630	-1.4595	-1.0526
C	2.4493	-1.1395	0.2145
C	1.5805	-1.2420	1.3027
C	0.2582	-1.6279	1.1294
C	-0.2216	-1.9248	-0.1420
C	0.6390	-1.8476	-1.2319
H	2.6220	-1.3762	-1.9072
H	1.9439	-1.0018	2.2953
H	-0.4061	-1.6880	1.9815
H	-1.2565	-2.2025	-0.2799
H	0.2756	-2.0804	-2.2248
C	3.8388	-0.5967	0.3930
H	4.4800	-0.9242	-0.4275
H	4.2745	-0.9700	1.3246
C	3.8538	0.9406	0.4353
H	3.2531	1.2823	1.2888
H	4.8789	1.2805	0.5992
O	3.4144	1.5336	-0.7663
H	2.4423	1.4877	-0.8068

Table S9. Equilibrium coordinates for isomer II (Ggπ+Ggπ-Lp+) of 2-phenylethanol dimer, according to the prediction with B3LYP-D3(BJ) /def2TZVP.

Atom	*a* / Å[a]	*b* / Å	*c* / Å
C	3.0756	-0.2666	-0.7134
C	2.2936	0.8028	-0.2723
C	1.8976	0.8304	1.0632
C	2.2810	-0.1791	1.9390
C	3.0594	-1.2379	1.4894
C	3.4554	-1.2798	0.1563
H	3.3971	-0.3019	-1.7481
H	1.2693	1.6394	1.4145
H	1.9666	-0.1390	2.9743
H	3.3579	-2.0238	2.1711
H	4.0655	-2.0988	-0.2029
C	1.8613	1.8838	-1.2285
H	1.4815	2.7410	-0.6695
H	2.7185	2.2321	-1.8132
C	0.7817	1.4243	-2.2093
H	1.1530	0.5998	-2.8262
H	0.5155	2.2463	-2.8750
O	-0.4245	1.0363	-1.5591
H	-0.3201	0.1485	-1.1883
C	-3.0083	-1.0860	-0.5120
C	-2.3602	-0.5752	0.6138
C	-1.0692	-1.0221	0.8920
C	-0.4286	-1.9338	0.0590
C	-1.0845	-2.4274	-1.0644
C	-2.3806	-2.0048	-1.3428
H	-4.0114	-0.7497	-0.7463
H	-0.5486	-0.6300	1.7540
H	0.5828	-2.2443	0.2851
H	-0.5903	-3.1364	-1.7160
H	-2.8994	-2.3862	-2.2130
C	-2.9924	0.4996	1.4533
H	-4.0702	0.3314	1.5370
H	-2.5759	0.4770	2.4624
C	-2.7711	1.9054	0.8701
H	-3.2577	2.6371	1.5193
H	-3.2451	1.9681	-0.1164
O	-1.4050	2.2626	0.7916
H	-1.0386	1.8944	-0.0325

Table S10. Equilibrium coordinates for isomer III (Ggπ-Ggπ-Lp-) of 2-phenylethanol dimer, according to the prediction with B3LYP-D3(BJ) /def2TZVP.

Atom	*a* / Å[a]	*b* / Å	*c* / Å
C	2.4665	0.5157	1.2782
C	2.4116	1.1394	0.0320
C	3.0559	0.5280	-1.0442
C	3.7411	-0.6687	-0.8809
C	3.7888	-1.2802	0.3674
C	3.1472	-0.6844	1.4461
H	1.9705	0.9772	2.1229
H	3.0262	1.0003	-2.0192
H	4.2414	-1.1231	-1.7266
H	4.3247	-2.2114	0.4977
H	3.1806	-1.1516	2.4222
C	1.6398	2.4179	-0.1579
H	2.1066	3.0216	-0.9409
H	1.6557	3.0063	0.7617
C	0.1802	2.1830	-0.5520
H	-0.3155	3.1408	-0.7135
H	0.1252	1.6097	-1.4827
O	-0.5622	1.5276	0.4720
H	-0.3061	0.5949	0.4991
C	-1.9031	-0.9907	-1.3866
C	-2.5215	-1.1278	-0.1447
C	-1.7602	-1.6046	0.9244
C	-0.4153	-1.9151	0.7621
C	0.1926	-1.7626	-0.4807
C	-0.5600	-1.3070	-1.5562
H	-2.4778	-0.6101	-2.2213
H	-2.2225	-1.7169	1.8982
H	0.1645	-2.2689	1.6046
H	1.2430	-1.9845	-0.6019
H	-0.0951	-1.1857	-2.5264
C	-3.9393	-0.6747	0.0641
H	-4.4583	-0.6239	-0.8948
H	-4.4790	-1.3872	0.6956
C	-4.0062	0.7098	0.7300
H	-5.0531	1.0039	0.8342
H	-3.5786	0.6483	1.7387
O	-3.3665	1.7141	-0.0279
H	-2.4076	1.6548	0.1326

Table S11. Equilibrium coordinates for isomer I (Ggπ- Ggπ+ Ggπ+ Lp-) of 2-phenylethanol trimer, according to the prediction with B3LYP-D3(BJ) /def2TZVP.

Atom	*a* / Åa	*b* / Å	*c* / Å
C	-0.8865	-3.6926	-0.0106
C	-2.0478	-3.1303	0.5059
C	-2.8075	-2.2322	-0.2438
C	-2.3656	-1.9008	-1.5246
C	-1.2071	-2.4614	-2.0469
C	-0.4643	-3.3624	-1.2927
C	-4.0576	-1.6174	0.3255
C	-3.8043	-0.2963	1.0466
O	-3.3503	0.6635	0.1156
H	-0.3181	-4.3972	0.5838
H	-2.3766	-3.4009	1.5028
H	-2.9395	-1.1969	-2.1126
H	-0.8876	-2.1996	-3.0478
H	0.4311	-3.8093	-1.7053
H	-4.5231	-2.3099	1.0315
H	-4.7795	-1.4340	-0.4737
H	-4.7361	0.0327	1.5257
H	-3.0639	-0.4519	1.8413
H	-2.8877	1.3764	0.6007
C	4.6274	-0.0178	0.6852
C	3.5133	-0.1124	1.5112
C	2.5192	-1.0598	1.2669
C	2.6666	-1.9078	0.1691
C	3.7796	-1.8202	-0.6563
C	4.7665	-0.8742	-0.4000
C	1.2973	-1.1403	2.1434
C	0.1458	-0.2659	1.6490
O	0.4881	1.1231	1.6413
H	5.3897	0.7222	0.8932
H	3.4119	0.5546	2.3583
H	1.8977	-2.6398	-0.0386
H	3.8787	-2.4918	-1.4998
H	5.6365	-0.8066	-1.0403
H	0.9352	-2.1703	2.1851
H	1.5495	-0.8373	3.1617
H	-0.1811	-0.5807	0.6561
H	-0.7026	-0.3596	2.3268
H	1.0788	1.2902	0.8930
C	2.0712	2.6041	-1.1735
C	0.9328	3.3725	-0.9649
C	-0.3415	2.8215	-1.1145

C	-0.4492	1.4858	-1.4995
C	0.6884	0.7166	-1.7175
C	1.9520	1.2685	-1.5472
C	-1.5654	3.6265	-0.7674
C	-1.7307	3.8022	0.7474
O	-1.8644	2.5665	1.4370
H	3.0520	3.0418	-1.0384
H	1.0342	4.4095	-0.6660
H	-1.4293	1.0341	-1.5816
H	0.5861	-0.3250	-1.9894
H	2.8348	0.6615	-1.6866
H	-2.4568	3.1393	-1.1660
H	-1.5072	4.6226	-1.2169
H	-0.8826	4.3641	1.1527
H	-2.6374	4.3736	0.9529
H	-0.9887	2.1288	1.5017
H	-0.9887	2.1288	1.5017

Table S12. Equilibrium coordinates for isomer II (E Ggπ+ Ggπ- Lp-) of 2-phenylethanol trimer, according to the prediction with B3LYP-D3(BJ) /def2TZVP.

Atom	*a* / Åa	*b* / Å	*c* / Å
C	-3.3128	-0.3479	-0.7519
C	-2.5468	-0.1405	0.3896
C	-3.9367	-1.5703	-0.9643
C	-2.3934	-1.1524	1.3363
C	-3.0199	-2.3792	1.1093
C	-1.5385	-0.9464	2.5594
C	-3.7871	-2.5890	-0.0284
C	-0.0949	-1.4095	2.3635
O	0.6014	-0.6164	1.4075
C	-1.2004	2.6753	-1.8551
C	-0.0410	2.5749	-1.0952
C	-0.0276	2.9710	0.2441
C	-1.2124	3.4646	0.7943
C	-2.3745	3.5618	0.0387
C	-2.3724	3.1680	-1.2939
C	1.2124	2.8739	1.0994
C	2.5450	3.1205	0.3873
O	2.9511	2.0561	-0.4578
C	0.4807	-3.3276	-0.9930
C	1.8357	-3.0821	-0.8138
C	2.3883	-1.8408	-1.1330
C	1.5529	-0.8551	-1.6571
C	0.1941	-1.0966	-1.8366
C	-0.3481	-2.3319	-1.4989
C	3.8297	-1.5405	-0.8223
C	4.0569	-1.2924	0.6743
O	3.3162	-0.1877	1.1732
H	-3.4188	0.4534	-1.4704
H	-2.0706	0.8183	0.5447
H	-4.5375	-1.7298	-1.8505
H	-2.9126	-3.1747	1.8377
H	-1.9577	-1.5015	3.4032
H	-1.5251	0.1099	2.8353
H	-4.2725	-3.5443	-0.1832
H	-0.0699	-2.4630	2.0665
H	0.4597	-1.3031	3.2965
H	0.2326	-0.7692	0.5247
H	-1.1859	2.3696	-2.8942
H	0.8687	2.1955	-1.5368
H	-1.2217	3.7824	1.8306

H	-3.2795	3.9488	0.4896
H	-3.2736	3.2482	-1.8882
H	1.1256	3.5946	1.9180
H	1.2483	1.8848	1.5672
H	2.4721	4.0088	-0.2440
H	3.3137	3.3169	1.1444
H	3.1510	1.2842	0.1067
H	0.0669	-4.2934	-0.7320
H	2.4724	-3.8603	-0.4086
H	1.9648	0.1184	-1.8878
H	-0.4463	-0.3128	-2.2174
H	-1.4076	-2.5090	-1.6153
H	4.1560	-0.6597	-1.3782
H	4.4682	-2.3756	-1.1260
H	5.1097	-1.0667	0.8515
H	3.8088	-2.1962	1.2415
H	2.3751	-0.4381	1.2764

Table S13. Equilibrium coordinates for isomer I (Gg+ At Gg- Ggπ+) of 2-phenylethanol tetramer, according to the prediction with B3LYP-D3(BJ) /def2TZVP.

Atom	*a* / Åa	*b* / Å	*c* / Å
C	2.6532	-0.8614	-3.3027
C	1.7922	0.0600	-2.7183
C	2.2768	1.0443	-1.8570
C	3.6460	1.0777	-1.5898
C	4.5113	0.1629	-2.1766
C	4.0167	-0.8106	-3.0381
C	1.3420	2.0317	-1.2129
C	0.8974	1.6337	0.1954
O	0.1781	0.4063	0.2263
C	1.9167	0.6133	3.5795
C	2.0157	-0.6279	2.9629
C	3.0930	-0.9309	2.1310
C	4.0669	0.0473	1.9257
C	3.9758	1.2877	2.5439
C	2.8991	1.5746	3.3759
C	3.1867	-2.2643	1.4391
C	2.5308	-2.2726	0.0564
O	1.1231	-2.0878	0.1314
C	-2.4185	3.4426	1.2865
C	-2.9799	2.5301	0.4045
C	-2.7469	2.6222	-0.9686
C	-1.9320	3.6529	-1.4312
C	-1.3707	4.5735	-0.5530
C	-1.6130	4.4722	0.8105
C	-3.3761	1.6420	-1.9280
C	-3.0106	0.1881	-1.6690
O	-1.6039	0.0251	-1.8137
C	-2.7553	-0.8059	2.0177
C	-2.0084	-1.8135	1.4202
C	-2.6300	-2.8346	0.7030
C	-4.0213	-2.8179	0.5926
C	-4.7733	-1.8171	1.1946
C	-4.1410	-0.8084	1.9139
C	-1.8199	-3.9250	0.0518
C	-1.5542	-3.7066	-1.4401
O	-0.7846	-2.5466	-1.7192
H	2.2551	-1.6210	-3.9633
H	0.7314	0.0183	-2.9296
H	4.0367	1.8314	-0.9166
H	5.5720	0.2105	-1.9635
H	4.6889	-1.5245	-3.4967

H	1.8244	3.0106	-1.1395
H	0.4542	2.1611	-1.8333
H	1.7618	1.4971	0.8421
H	0.2788	2.4306	0.6149
H	-0.5392	0.4214	-0.4454
H	1.0699	0.8299	4.2179
H	1.2463	-1.3720	3.1246
H	4.9055	-0.1685	1.2749
H	4.7457	2.0306	2.3774
H	2.8253	2.5406	3.8582
H	4.2370	-2.5423	1.3138
H	2.7151	-3.0370	2.0503
H	2.9799	-1.5085	-0.5786
H	2.6976	-3.2420	-0.4177
H	0.9070	-1.1258	0.2139
H	-2.6099	3.3517	2.3483
H	-3.6035	1.7326	0.7854
H	-1.7349	3.7353	-2.4933
H	-0.7401	5.3661	-0.9355
H	-1.1755	5.1849	1.4976
H	-4.4663	1.7250	-1.8714
H	-3.0889	1.8991	-2.9495
H	-3.5356	-0.4467	-2.3907
H	-3.3261	-0.1168	-0.6682
H	-1.3922	-0.9374	-1.8201
H	-2.2473	-0.0151	2.5536
H	-0.9312	-1.8048	1.5049
H	-4.5220	-3.6050	0.0403
H	-5.8524	-1.8268	1.1071
H	-4.7264	-0.0302	2.3872
H	-0.8608	-4.0245	0.5639
H	-2.3400	-4.8822	0.1536
H	-1.0504	-4.5921	-1.8452
H	-2.4978	-3.5891	-1.9770
H	-0.0086	-2.4997	-1.1123

Table S14. Equilibrium coordinates for isomer II (Ggπ+ Gg+ Ggπ+ Gt) of 2-phenylethanol tetramer, according to the prediction with B3LYP-D3(BJ) /def2TZVP.

Atom	*a* / Åa	*b* / Å	*c* / Å
C	-5.6477	-0.5752	0.1300
C	-4.7592	-0.7669	-0.9202
C	-3.9963	0.2901	-1.4180
C	-4.1391	1.5453	-0.8269
C	-5.0239	1.7419	0.2263
C	-5.7845	0.6826	0.7067
C	-3.0176	0.0687	-2.5397
C	-1.6156	-0.3047	-2.0541
O	-0.9845	0.7638	-1.3555
C	4.1749	-3.7048	-1.0515
C	4.2153	-2.3548	-1.3772
C	3.9347	-1.3774	-0.4222
C	3.6132	-1.7873	0.8703
C	3.5708	-3.1358	1.2014
C	3.8514	-4.1001	0.2415
C	3.9273	0.0811	-0.7988
C	2.6306	0.5072	-1.4774
O	1.5552	0.2646	-0.5861
C	-2.0898	-3.7502	-0.4107
C	-2.3840	-2.9458	0.6826
C	-1.3893	-2.1834	1.2975
C	-0.0947	-2.2430	0.7859
C	0.2048	-3.0400	-0.3124
C	-0.7923	-3.7993	-0.9120
C	-1.7143	-1.2995	2.4729
C	-2.3095	0.0563	2.0876
O	-1.4245	0.8631	1.3181
C	0.6609	3.7465	-1.3841
C	0.5335	3.4400	-0.0347
C	1.6104	3.5904	0.8364
C	2.8222	4.0564	0.3230
C	2.9515	4.3753	-1.0223
C	1.8680	4.2213	-1.8813
C	1.4881	3.2173	2.2898
C	2.0034	1.8092	2.6023
O	1.2287	0.7824	2.0034
H	-6.2355	-1.4072	0.4972
H	-4.6539	-1.7498	-1.3628
H	-3.5467	2.3733	-1.1948
H	-5.1178	2.7234	0.6730
H	-6.4771	0.8351	1.5242

H	-3.3741	-0.7387	-3.1852
H	-2.9412	0.9688	-3.1538
H	-0.9845	-0.5300	-2.9161
H	-1.6570	-1.1968	-1.4282
H	-1.2910	0.7754	-0.4196
H	4.3973	-4.4482	-1.8065
H	4.4693	-2.0547	-2.3875
H	3.3738	-1.0439	1.6201
H	3.3065	-3.4336	2.2079
H	3.8141	-5.1510	0.4971
H	4.0724	0.6991	0.0905
H	4.7541	0.3013	-1.4788
H	2.6806	1.5668	-1.7414
H	2.4877	-0.0731	-2.3964
H	0.6871	0.4814	-0.9993
H	-2.8721	-4.3411	-0.8710
H	-3.3967	-2.9078	1.0654
H	0.6881	-1.6574	1.2456
H	1.2174	-3.0633	-0.6911
H	-0.5621	-4.4259	-1.7643
H	-0.8125	-1.1321	3.0668
H	-2.4379	-1.7984	3.1242
H	-3.2045	-0.0787	1.4836
H	-2.5993	0.5935	2.9980
H	-0.5273	0.8604	1.7168
H	-0.1828	3.5973	-2.0444
H	-0.4097	3.0679	0.3437
H	3.6697	4.1817	0.9874
H	3.8963	4.7450	-1.4005
H	1.9671	4.4663	-2.9311
H	2.0553	3.9231	2.9040
H	0.4444	3.2801	2.6051
H	3.0498	1.7197	2.2896
H	1.9659	1.6411	3.6806
H	1.4697	0.6718	1.0504

Table S15. Equilibrium coordinates for isomer III (Gt Gg+ Gt Gg-) of 2-phenylethanol tetramer, according to the prediction with B3LYP-D3(BJ) /def2TZVP.

Atom	*a* / Åa	*b* / Å	*c* / Å
C	-5.3687	1.9654	0.0332
C	-4.7299	1.3210	1.0870
C	-4.2926	0.0038	0.9660
C	-4.5018	-0.6529	-0.2477
C	-5.1331	-0.0131	-1.3052
C	-5.5739	1.2992	-1.1680
C	-3.6233	-0.6966	2.1233
C	-2.2440	-1.2526	1.8035
O	-1.3921	-0.1846	1.4059
C	1.7977	2.9494	1.5612
C	0.4776	2.6433	1.2532
C	-0.2085	3.3509	0.2665
C	0.4654	4.3680	-0.4112
C	1.7835	4.6811	-0.1037
C	2.4538	3.9736	0.8886
C	-1.6388	3.0179	-0.0663
C	-1.8055	2.1031	-1.2812
O	-1.1930	0.8308	-1.1155
C	-1.7977	-2.9496	-1.5611
C	-0.4777	-2.6435	-1.2531
C	0.2085	-3.3511	-0.2664
C	-0.4655	-4.3682	0.4113
C	-1.7836	-4.6812	0.1038
C	-2.4539	-3.9736	-0.8885
C	1.6388	-3.0181	0.0662
C	1.8056	-2.1032	1.2810
O	1.1930	-0.8309	1.1153
C	5.3689	-1.9650	-0.0328
C	4.7301	-1.3209	-1.0867
C	4.2926	-0.0037	-0.9659
C	4.5016	0.6531	0.2477
C	5.1330	0.0135	1.3053
C	5.5740	-1.2987	1.1682
C	3.6233	0.6965	-2.1234
C	2.2440	1.2524	-1.8038
O	1.3920	0.1845	-1.4061
H	-5.7011	2.9890	0.1508
H	-4.5687	1.8483	2.0196
H	-4.1605	-1.6725	-0.3673
H	-5.2824	-0.5393	-2.2396

H	-6.0682	1.7977	-1.9918
H	-3.5382	-0.0043	2.9633
H	-4.2489	-1.5303	2.4584
H	-1.8386	-1.7421	2.6952
H	-2.3038	-2.0036	1.0129
H	-0.4603	-0.5085	1.3570
H	2.3119	2.3801	2.3246
H	-0.0291	1.8480	1.7828
H	-0.0530	4.9299	-1.1800
H	2.2858	5.4806	-0.6336
H	3.4794	4.2196	1.1333
H	-2.1156	2.5386	0.7897
H	-2.1979	3.9360	-0.2692
H	-2.8711	1.9735	-1.4869
H	-1.3416	2.5548	-2.1607
H	-1.4488	0.4484	-0.2454
H	-2.3119	-2.3803	-2.3245
H	0.0291	-1.8482	-1.7828
H	0.0529	-4.9301	1.1800
H	-2.2859	-5.4807	0.6337
H	-3.4795	-4.2197	-1.1332
H	2.1979	-3.9363	0.2692
H	2.1156	-2.5390	-0.7898
H	2.8712	-1.9736	1.4865
H	1.3418	-2.5548	2.1607
H	1.4487	-0.4485	0.2452
H	5.7015	-2.9887	-0.1503
H	4.5691	-1.8483	-2.0193
H	4.1602	1.6727	0.3671
H	5.2821	0.5399	2.2396
H	6.0683	-1.7971	1.9921
H	4.2490	1.5302	-2.4586
H	3.5383	0.0040	-2.9633
H	2.3036	2.0036	-1.0134
H	1.8387	1.7418	-2.6957
H	0.4603	0.5084	-1.3573

Table S16. Equilibrium coordinates for isomer IV (Gg- Gg- Ggπ+ Ggπ-) of 2-phenylethanol tetramer, according to the prediction with B3LYP-D3(BJ) /def2TZVP.

Atom	*a* / Åa	*b* / Å	*c* / Å
C	-4.5785	-0.4306	-0.0214
C	-3.4511	-0.0631	-0.7439
C	-2.9674	-0.8768	-1.7686
C	-3.6436	-2.0630	-2.0510
C	-4.7720	-2.4347	-1.3304
C	-5.2436	-1.6175	-0.3098
C	-1.7195	-0.5115	-2.5247
C	-0.4268	-0.7848	-1.7495
O	-0.2742	0.0700	-0.6282
C	-1.8167	-2.8667	0.9024
C	-0.9707	-2.1688	1.7551
C	0.3686	-2.5292	1.8904
C	0.8476	-3.6007	1.1346
C	0.0077	-4.3016	0.2791
C	-1.3301	-3.9379	0.1647
C	1.2927	-1.7641	2.8018
C	2.1634	-0.7495	2.0627
O	1.4011	0.3105	1.4975
C	-3.6204	2.9904	1.2107
C	-2.7625	3.7252	0.4023
C	-1.3778	3.6052	0.5313
C	-0.8736	2.7218	1.4838
C	-1.7280	1.9739	2.2836
C	-3.1039	2.1107	2.1556
C	-0.4513	4.3942	-0.3558
C	-0.1362	3.7121	-1.6896
O	0.5636	2.4828	-1.5477
C	3.0493	-1.7341	-1.3784
C	3.2045	-0.3555	-1.4564
C	4.3232	0.2700	-0.9072
C	5.2803	-0.5213	-0.2705
C	5.1336	-1.9009	-0.1963
C	4.0164	-2.5119	-0.7536
C	4.4876	1.7649	-0.9739
C	3.9297	2.5063	0.2451
O	2.5146	2.4505	0.3328
H	-4.9351	0.2129	0.7717
H	-2.9353	0.8541	-0.4991
H	-3.2785	-2.7058	-2.8437
H	-5.2826	-3.3600	-1.5659

H	-6.1225	-1.9021	0.2545
H	-1.6776	-1.0787	-3.4585
H	-1.7349	0.5475	-2.7982
H	0.4212	-0.6705	-2.4338
H	-0.4231	-1.8045	-1.3669
H	-0.1122	0.9830	-0.9530
H	-2.8486	-2.5634	0.8006
H	-1.3537	-1.3238	2.3129
H	1.8883	-3.8893	1.2226
H	0.3955	-5.1346	-0.2940
H	-1.9892	-4.4774	-0.5029
H	0.7150	-1.2382	3.5647
H	1.9594	-2.4599	3.3198
H	2.8557	-0.2820	2.7653
H	2.7520	-1.2495	1.2911
H	0.8083	-0.0145	0.7817
H	-4.6916	3.1020	1.0998
H	-3.1730	4.4092	-0.3319
H	0.1950	2.6137	1.6021
H	-1.3104	1.2845	3.0055
H	-3.7697	1.5333	2.7840
H	0.4894	4.5838	0.1667
H	-0.8941	5.3683	-0.5827
H	-1.0615	3.4787	-2.2201
H	0.4444	4.3981	-2.3173
H	1.3405	2.6002	-0.9556
H	2.1688	-2.2021	-1.7966
H	2.4497	0.2464	-1.9455
H	6.1574	-0.0520	0.1602
H	5.8925	-2.4981	0.2930
H	3.8973	-3.5861	-0.6982
H	5.5494	2.0141	-1.0575
H	3.9936	2.1562	-1.8662
H	4.3771	2.1085	1.1618
H	4.1997	3.5623	0.1758
H	2.2177	1.6229	0.7858