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

Torsional Chirality and Molecular Recognition: The Homo and Heterochiral Dimers of Thenyl and Furfuryl Alcohol

ELECTRONIC SUPPLEMENTARY INFORMATION

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1. Supplementary Figures

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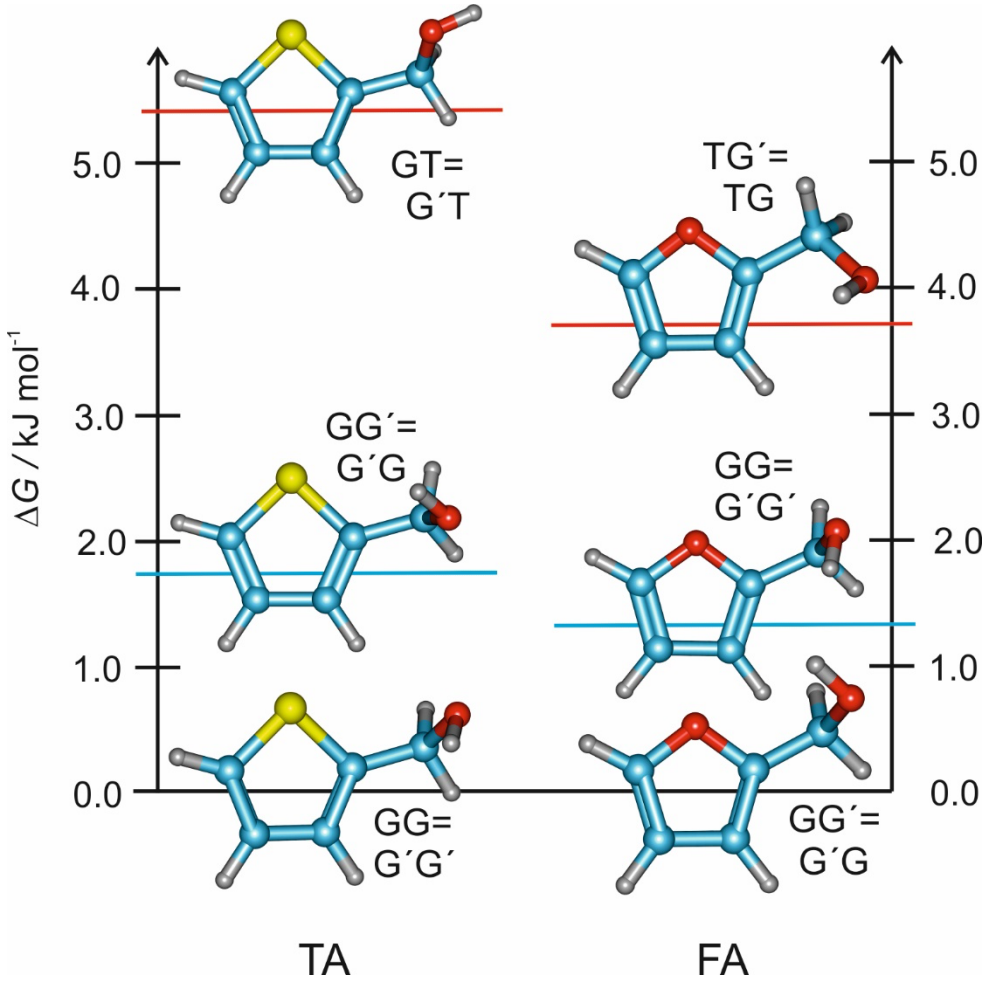

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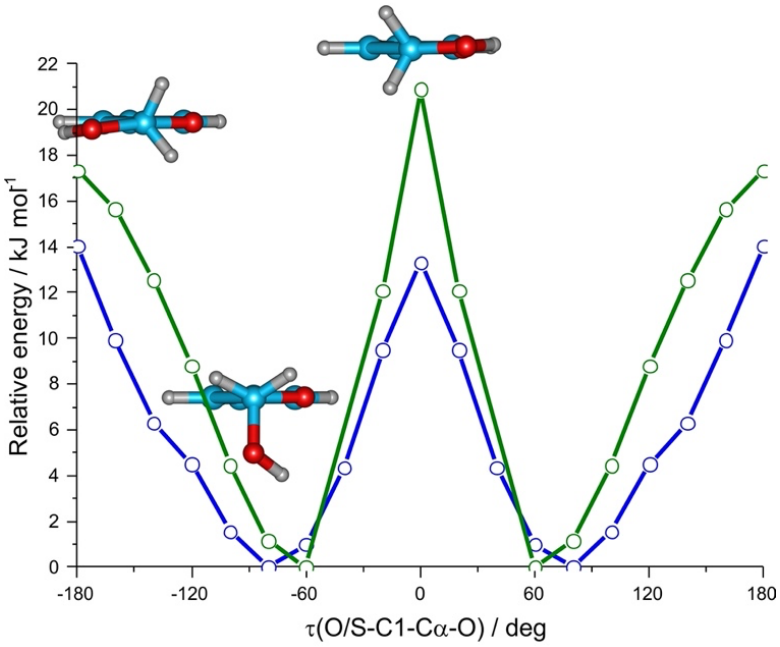

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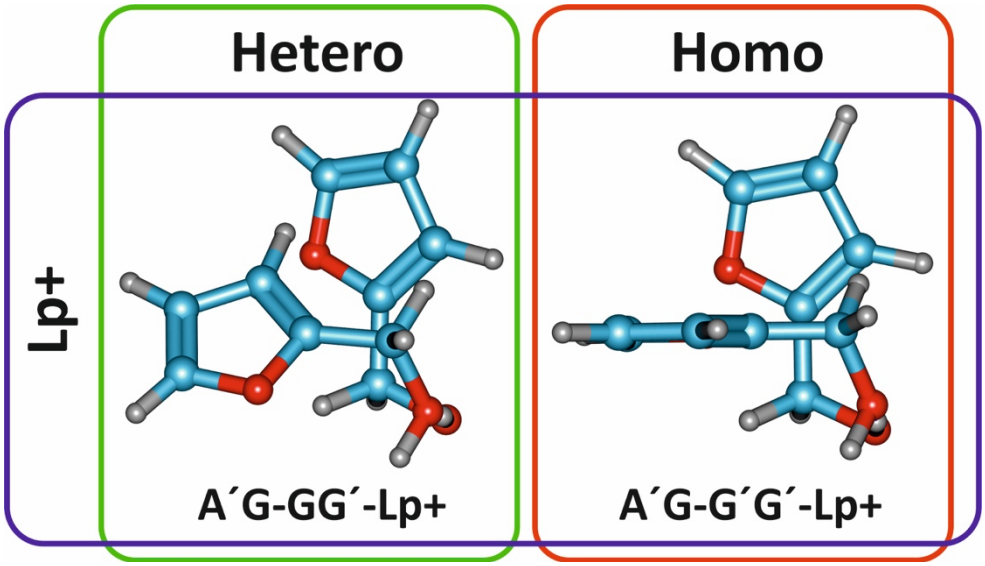

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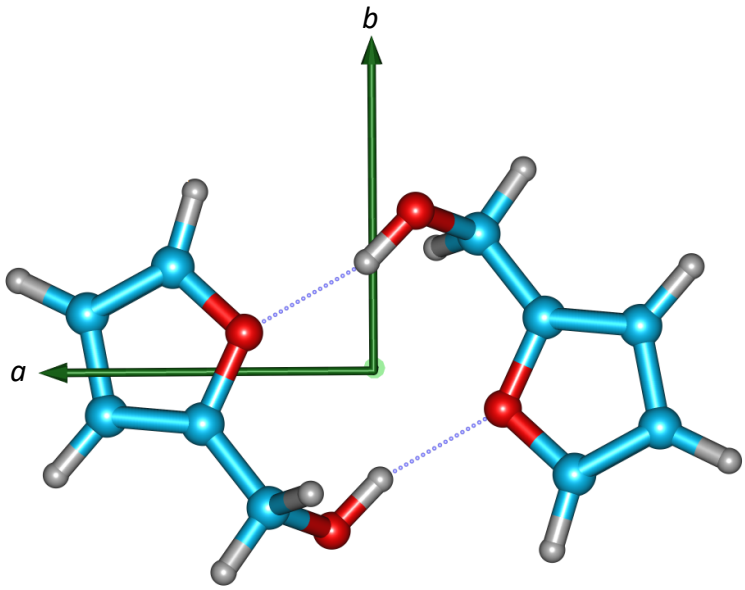

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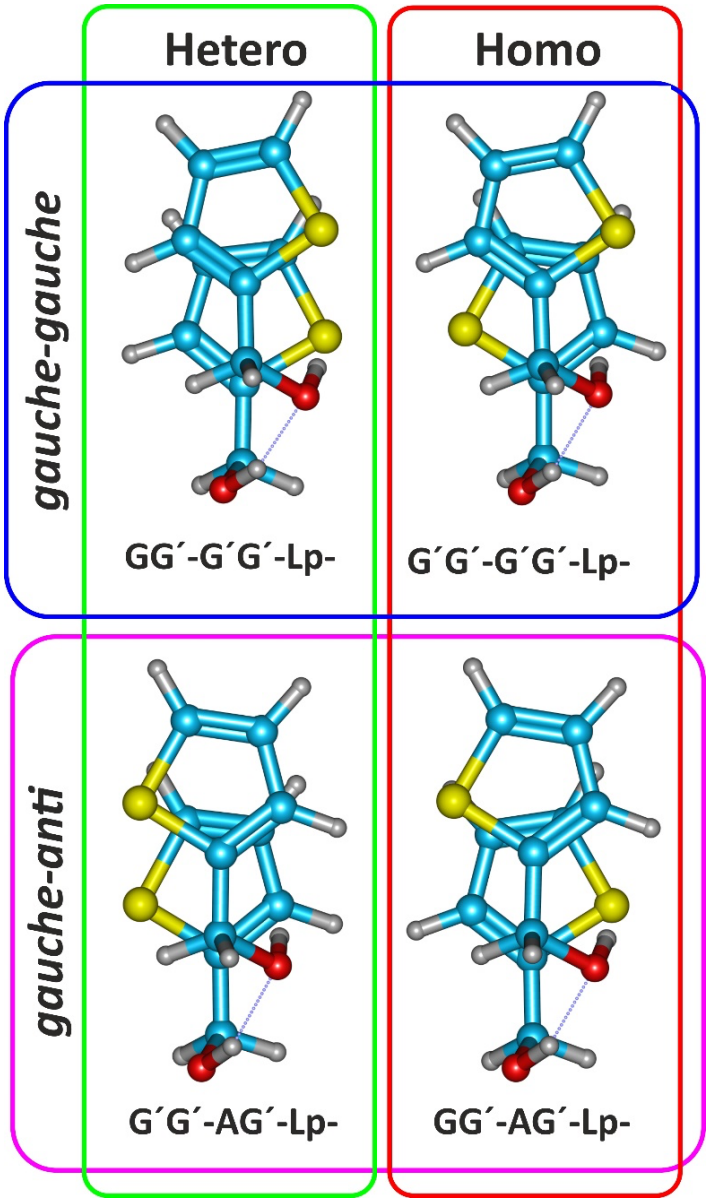

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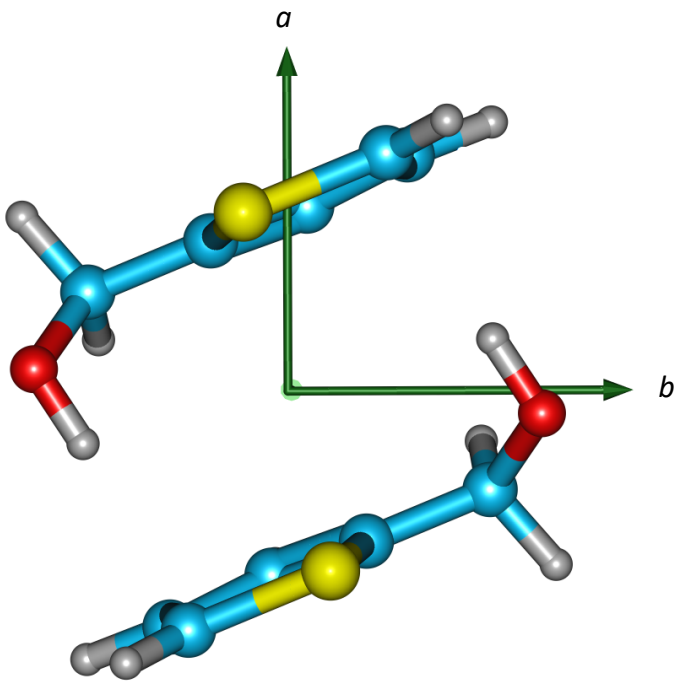

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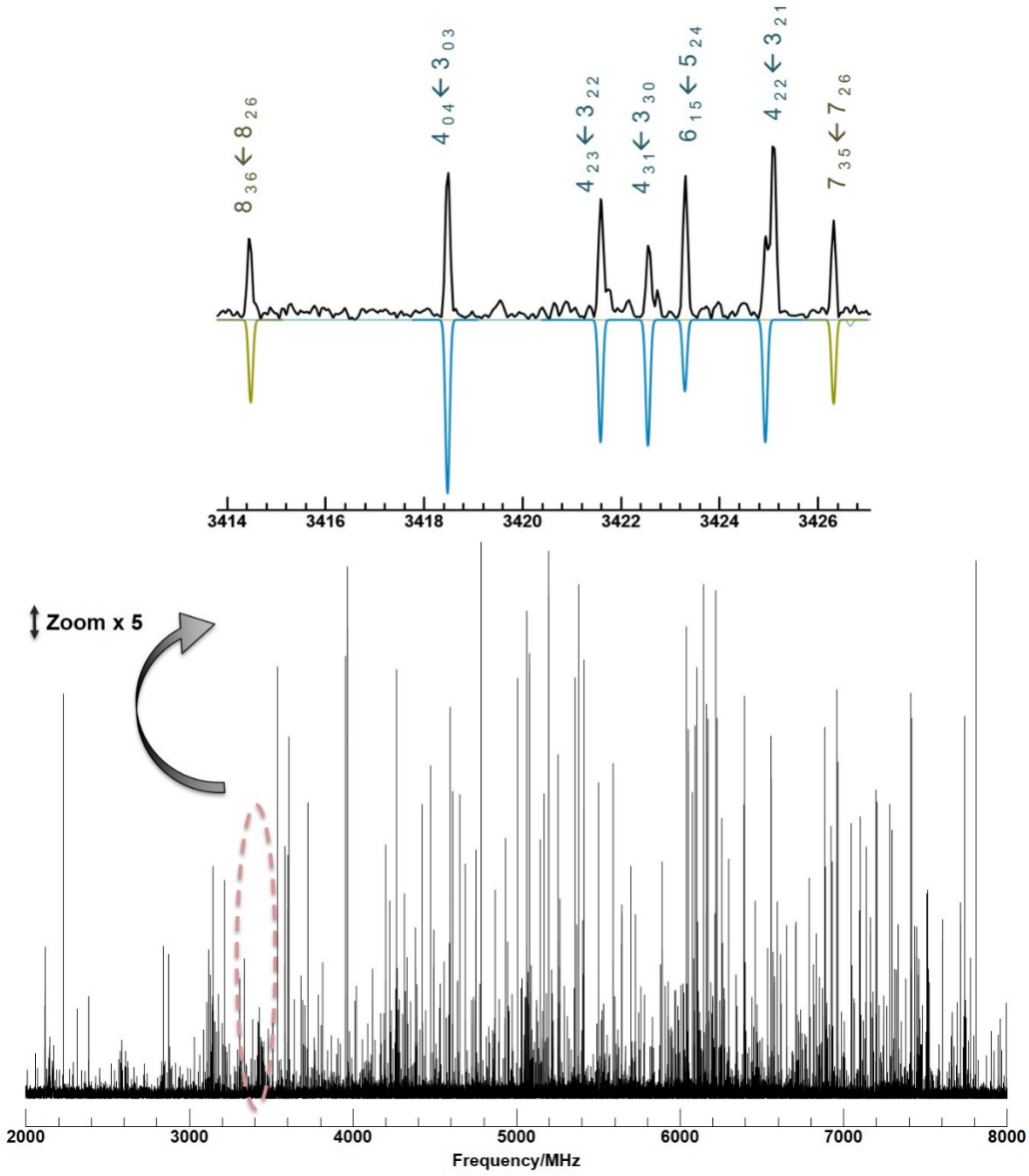

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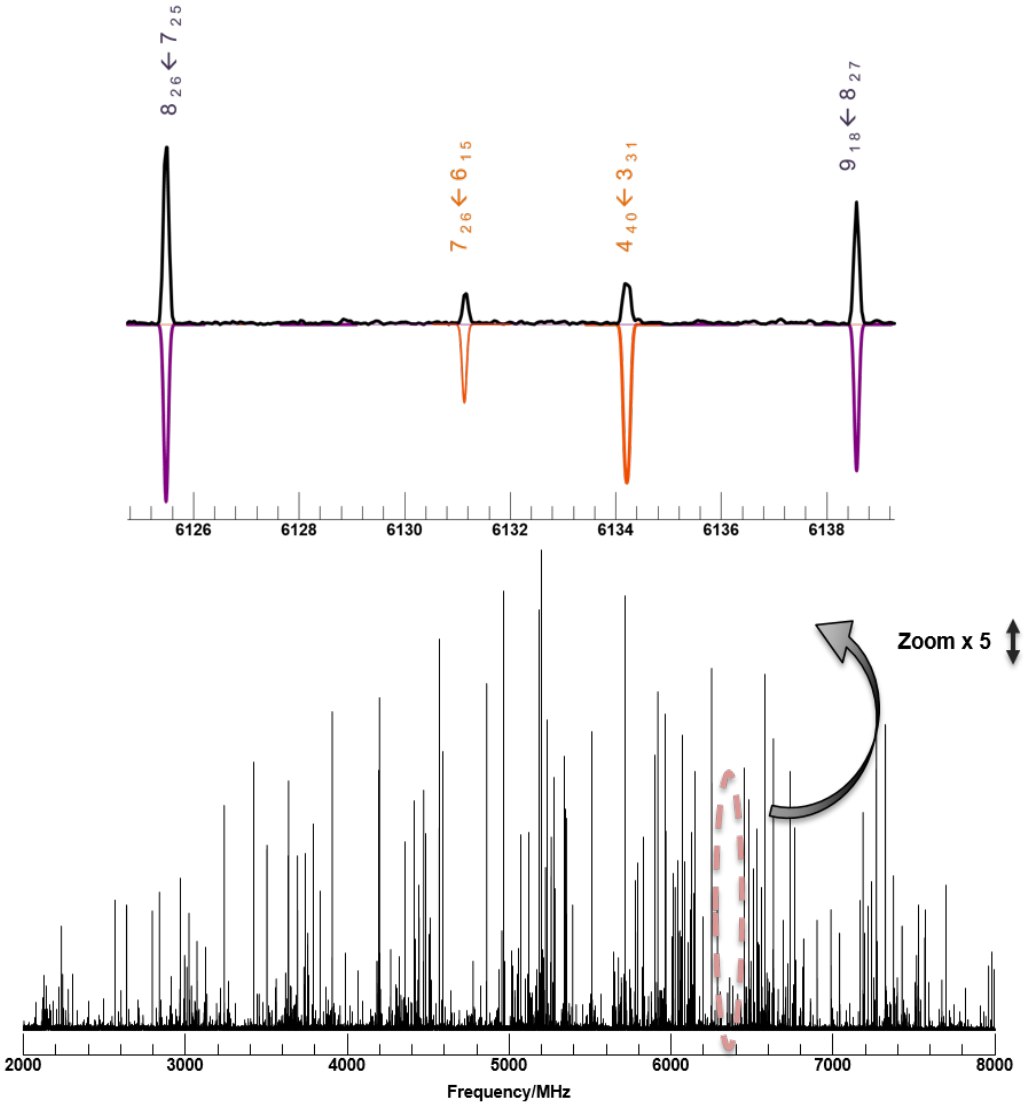

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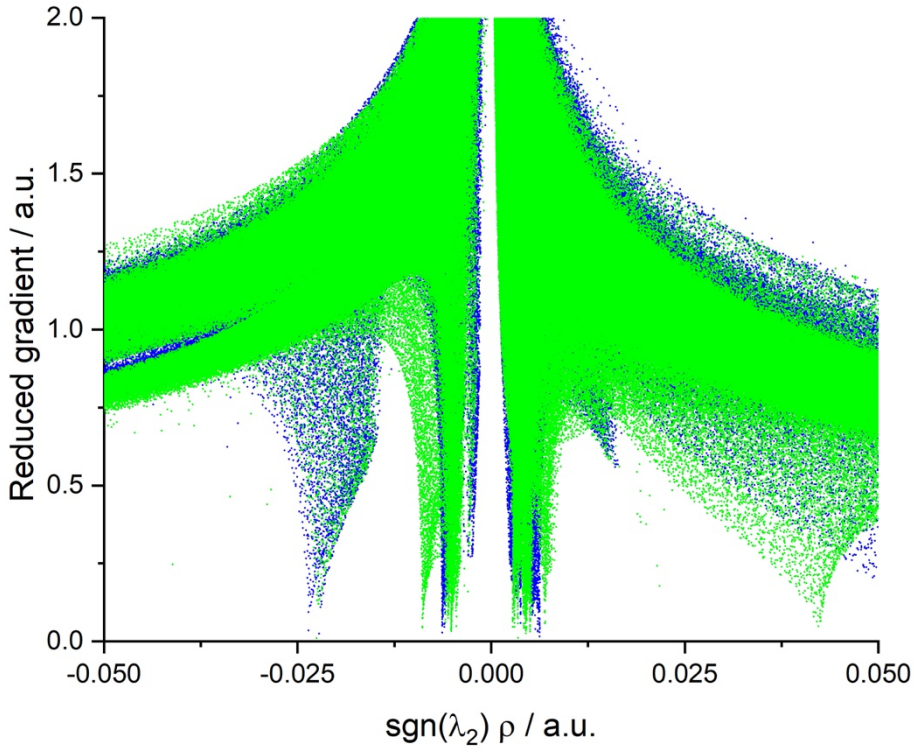
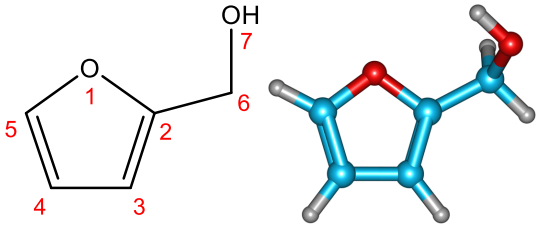


2. Supplementary Tables

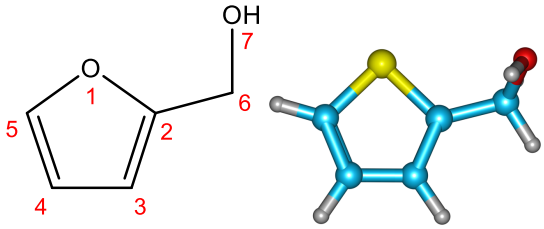
Table S1. Computational predictions for the optimized structure of furfuryl alcohol GG´ in the principal inertial axis system (B3LYP-D3(BJ) and MP2, basis set 6-311++G(d,p)).



Furfuryl Alcohol GG´ [a]			
	Theory [b]		
	a / Å [c]	***b*** / Å	***c*** / Å
O (1)	0.4042/0.3860[b]	-0.9880/-0.9852	0.2307/0.2350
C (2)	-0.1692/-0.1685	0.2597/0.2656	0.2426/0.2416
C (3)	0.7739/0.7917	1.1955/1.2009	-0.0508/-0.0553
C (4)	2.0066/2.0122	0.4902/0.4812	-0.2551/-0.2553
C (5)	1.7234/1.7047	-0.8260/-0.8415	-0.0776/-0.0716
C (6)	-1.6271/-1.6285	0.3083/0.3269	0.5234/0.5171
O (7)	-2.4327/-2.4202	-0.1748/-0.1825	-0.5571/-0.5572
H (3)	0.6099/0.6320	2.2590/2.2674	-0.1195/-0.1265
H (4)	2.9687/2.9857	0.9097/0.8799	-0.5015/-0.5017
H (5)	2.3106/2.2800	-1.7269/-1.7536	-0.1261/-0.1164
H (6)	-1.9235/-1.9189	1.3454/1.3718	0.6793/0.6396
H (6')	-1.8482/-1.8554	-0.2523/-0.2105	1.4407/1.44701
H (7)	-2.1646/-2.1270	-1.0801/-1.0858	-0.7472/-0.7116

[a]Juanes et al., *Chem. - A Eur. J.* 2018, *24*, 6564–6571. [b]B3LYP-D3(BJ) / MP2 coordinates, respectively (basis set 6-311++G(d,p)). [c]Principal inertial axes denoted *a*, *b*, *c*.

Table S2. Computational predictions for the optimized structure of thenyl alcohol GG in the principal inertial axis system (B3LYP-D3(BJ) and MN15-L, basis set def2TZVP).



Thenyl Alcohol GG [a]			
Theory [b]			
	a / Å [c]	***b*** / Å	***c*** / Å
S(1)	0.4858/ 0.3974	-1.1377/-1.1157	-0.1240/-0.1298
C(2)	-0.3426/-0.3232	0.3794/ 0.4485	-0.2276/-0.1669
C(3)	0.5271/ 0.6300	1.4164/ 1.4260	-0.0273/ 0.0205
C(4)	1.8643/ 1.9464	0.9934/ 0.8984	0.2043/ 0.1836
C(5)	1.9897/ 1.9648	-0.3649/-0.4752	0.1810/ 0.1259
C(6)	-1.8115/-1.8020	0.45611/ 0.6160	-0.4869/-0.3900
O(7)	-2.5990/-2.5843	-0.1872/-0.2550	0.5131/ 0.4107
H(3)	2.8797/ 2.8177	-0.9527/-1.1427	0.3355/ 0.2398
H(4)	2.6902/ 2.8373	1.6661/ 1.5074	0.3839/ 0.3496
H(5)	0.2153/ 0.3833	2.4517/ 2.4910	-0.0501/ 0.0393
H(6)	-2.0768/-2.0799	-0.0434/ 0.3765	-1.4198/-1.4327
H(6')	-2.0846/-2.0527	1.5131/ 1.6857	-0.5872/-0.2182
H(7)	-2.3043/-2.2638	0.1310/-0.1683	1.3743/ 1.3208

[a]Juanes et al., *Phys. Chem. Chem. Phys.* 2020, *22*, 12412–12421. [b]B3LYP-D3(BJ) / MN15-L coordinates, respectively (basis set def2-TZVP). [c]Principal inertial axes denoted *a*, *b*, *c*.

Table S3. Computational predictions (B3LYP-D3(BJ) and MP2, basis set def2TZVP) for the most stable conformations of furfuryl alcohol.

	Theory[c]		
	GG´	GG	TG´
A / MHz[a]	6978.82/6931.13	6971.77/6900.57	7331.93/7216.27
B / MHz	1935.13/1947.23	1919.06/1932.27	1925.40/1923.85
C / MHz	1654.91/1659.48	1656.54/1666.07	1569.06/1581.30
D_J / kHz	0.3756/0.3429	0.3106/0.3530	0.1699/0.2193
D_{JK} / kHz	4.535/3.088	1.326/1.064	1.350/6.404
D_K / kHz	1.31/3.45	4.48/0.59	2.25/0.52
d_1 / kHz	-0.0510/-0.0294	-0.0136/-0.0067	-0.0352/-0.0314
d_2 / kHz	0.0073/0.0020	0.0103/0.0115	-0.0142/-0.0450
$\lvert\mu_a\rvert$ / D	1.67/1.66	1.71/1.71	1.27/1.44
$\lvert\mu_b\rvert$ / D	0.17/0.20	1.78/1.72	0.07/0.14
$\lvert\mu_c\rvert$ / D	0.66/0.75	0.14/0.06	0.83/0.65
ΔE / kJ mol^{-1} [b]	0.00/0.00	1.33/0.96	3.63/4.89
ΔG / kJ mol^{-1}	0.00/0.00	2.17/1.33	3.94/3.76

[a]Rotational constants (A, B, C), 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). [b]Relative energies corrected with the zero-point energy (ZPE) and Gibbs energy (ΔG, 298K, 1 atm). [c]B3LYP-D3(BJ) / MP2 values, respectively (basis set 6-311++G(d,p)).

Table S4. Computational predictions (B3LYP-D3(BJ) and MN15-L, basis set def2TZVP) for the most stable conformations of thenyl alcohol.

	Theory[c]		
	GG	GG'	GT
A / MHz[a]	4619.71/4699.21	4528.70/4521.34	4694.52/4766.17
B / MHz	1728.88/1750.34	1696.59/1700.30	1744.64/1770.48
C / MHz	1349.57/1343.48	1347.55/1352.55	1348.01/1344.52
D_J / kHz	0.182/0.174	0.256/0.295	0.179/0.164
D_{JK} / kHz	5.033 /3.985	6.066/7.979	6.545/3.092
D_K / kHz	-2.377/-1.600	-4.694/-6.623	-3.480/-1.168
d_1 / kHz	-0.044/-0.065	-0.024/-0.036	0.070/-0.068
d_2 / kHz	-0.016/-0.029	0.014 /0.022	0.037/-0.029
$\lvert\mu_a\rvert$ / D	1.36/1.26	1.50/1.43	0.69/0.83
$\lvert\mu_b\rvert$ / D	1.43/1.27	0.27/0.15	0.93/1.13
$\lvert\mu_c\rvert$ / D	0.34/0.62	0.10/0.10	1.24/0.99
ΔE/kJmol^{-1} [b]	0.0/0.0	2.42/3.69	6.13/5.76
ΔG/kJmol^{-1}	0.0/0.0	1.91/2.64	5.63/5.85

[a]Rotational constants (A, B, C), 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). [b]Relative energies corrected with the zero-point energy (ZPE) and Gibbs energy (ΔG, 298K, 1 atm). [c]B3LYP-D3(BJ) / MN15-L calculations, respectively (basis set def2TZVP).

Table S5. Conformational search and predicted rotational parameters for the dimer of (furfuryl alcohol)$_2$ using B3LYP-D3(BJ)/def2-TZVP. The isomers observed experimentally are marked in bold characters.

	Isomers							
	O-H···O-H···O$_r$				O-H···O-H···π			
	G´G-GG´ Lp+	G´G-G´G´- Lp+	**G´G-GG- Lp-**	**G´G-G´G- Lp-**	G´G´-GG´- Lp+	G´G´-G´G´- Lp+	G´G´-GG- Lp-	G´G´-G´G- Lp-
A / MHz[a]	881.29	914.57	**1099.63**	**1056.72**	1002.30	994.54	913.10	934.85
B / MHz	639.35	609.60	**422.05**	**442.06**	484.53	471.72	585.51	571.46
C / MHz	477.69	450.82	**409.19**	**427.87**	449.10	429.42	509.70	487.20
D_J / kHz	0.227	0.283	**0.159**	**0.187**	0.318	0.134	0.162	0.160
D_{JK} / kHz	-0.252	-0.311	**-0.689**	**-0.659**	-0.398	0.021	0.148	-0.104
D_K / kHz	0.165	0.199	**1.758**	**1.429**	0.493	0.003	-0.021	0.297
d_1 / kHz	0.031	0.032	**0.016**	**-0.032**	-0.025	0 .002	-0.017	-0.026
d_2 / kHz	0.005	0.010	**-0.001**	**0.000**	-0.003	-0.001	-0.005	-0.002
$\lvert\mu_a\rvert$ / D	0.6	1.7	**0.0**	**0.8**	1.9	2.7	0.8	0.9
$\lvert\mu_b\rvert$ / D	2.7	2.8	**0.2**	**2.6**	3.0	3.8	2.9	2.1
$\lvert\mu_c\rvert$ / D	0.5	1.5	**3.7**	**1.3**	0.1	0.6	2.1	1.2
ΔE / kJ mol^{-1} [b]	0.0	1.6	**2.3**	**0.8**	1.6	2.2	2.3	1.4
ΔG / kJ mol^{-1}	0.3	1.5	**1.9**	**0.2**	0.2	1.8	2.7	0.4
ΔE_C / kJ mol^{-1}	-45.3	-41.9	**-42.7**	**-42.5**	-42.4	-40.9	-40.4	-43.4
$\Delta\Delta E_C$ / kJ mol^{-1}	0.0	3.4	**2.6**	**2.8**	2.9	4.4	4.9	1.9

[a]Rotational constants (A, B, C), 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). [b]Relative energies corrected with the zero-point energy (ΔE), Gibbs energy (ΔG, 298K, 1 atm) and complexation energy including BSSE corrections (ΔE_B) relative to the monomers in the geometry of the dimer.

Table S6. Conformational search and predicted rotational parameters for the dimer of (furfuryl alcohol)$_2$ using B2PLYP-D3(BJ)/def2-TZVP. The isomers observed experimentally are marked in bold characters.

	Isomers							
	O-H···O-H···O$_r$				O-H···O-H···π			
	G′G-GG′ Lp+	G′G-G′G′-Lp+	G′G-GG-Lp-	G′G-G′G-Lp-	G′G′-GG′-Lp+	G′G′-G′G′-Lp+	G′G′-G′G-Lp-	G′G′-GG-Lp-
A / MHz[a]	877.91	913.35	**1096.27**	**1055.02**	991.62	991.96	918.68	940.81
B / MHz	641.07	611.25	**421.88**	**443.70**	498.43	473.15	582.83	568.38
C / MHz	477.02	451.29	**409.86**	**427.77**	459.90	429.25	508.80	487.15
D_J / kHz	0.242	0.295	**0.159**	**0.198**	0.481	0.153	0.173	0.175
D_{JK} / kHz	-0.284	-0.333	**-0.667**	**-0.676**	-0.687	-0.007	0.028	-0.156
D_K / kHz	0.178	0.206	**1.692**	**1.461**	0.506	0.006	0.113	0.424
d_1 / kHz	0.030	0.036	**0.018**	**-0.029**	-0.013	0.006	-0.020	-0.027
d_2 / kHz	0.017	0.016	**-0.002**	**0.002**	-0.002	-0.002	-0.004	-0.001
$\lvert\mu_a\rvert$ / D	0.6	1.7	**0.1**	**0.9**	2.0	2.8	0.9	0.9
$\lvert\mu_b\rvert$ / D	2.7	2.8	**0.3**	**2.6**	3.0	3.8	2.9	2.1
$\lvert\mu_c\rvert$ / D	0.5	1.6	**3.8**	**1.3**	0.1	0.6	2.1	1.2
ΔE / kJ mol^{-1} [b]	0.0	1.3	**2.2**	**0.7**	1.5	2.0	1.7	1.1
ΔG / kJ mol^{-1}	0.2	1.3	**2.1**	**0.1**	0.1	1.7	2.4	0.0
ΔE_B / kJ mol^{-1}	-40.8	-38.4	**-39.2**	**-38.9**	-38.8	-37.4	-37.1	-39.5
$\Delta\Delta E_B$ / kJ mol^{-1}	0.0	2.4	**1.6**	**1.9**	2.0	3.4	3.7	1.3

[a]Rotational constants (A, B, C), 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). [b]Relative energies corrected with the zero-point energy (ΔE), Gibbs energy (ΔG, 298K, 1 atm) and complexation energy including BSSE corrections (ΔE_B) relative to the monomers in the geometry of the dimer.

Table S7. Conformational search and predicted rotational parameters for the dimer (thenyl alcohol)$_2$ using B3LYP-D3(BJ)/def2-TZVP. The isomers observed experimentally are marked in bold characters.

	Isomers											
	O-H···O-H···π				O-H···O-H···π				O-H···O, π···π			
	G´G´-GG´-Lp+	**G´G´-G´G´-Lp+**	G´G´-GG-Lp-	G´G´-G´G-Lp-	A´G-GG´-Lp+	A´G-G´G´-Lp+	A´G-GG-Lp-	A´G-G´G-Lp-	GG´-G´G´-Lp-	G´G´-G´G´-Lp-	G´G´-AG´-Lp-	GG´-AG´-Lp-
A / MHz[a]	**833.26**	766.50	745.10	748.39	743.78	745.52	721.32	715.90	834.04	874.89	882.52	845.23
B / MHz	**381.90**	438.54	470.30	459.67	450.41	453.47	468.02	461.37	417.26	406.41	400.75	409.30
C / MHz	**347.94**	386.29	408.63	403.11	394.13	394.78	400.59	397.61	356.53	350.53	355.69	357.42
D_J / kHz	**0.115**	0.170	0.065	0.070	0.098	0.096	0.071	0.088	0.145	0.087	0.085	0.114
D_{JK} / kHz	**-0.214**	-0.458	0.055	0.102	0.076	0.139	0.094	0.222	0.211	-0.073	-0.106	-0.242
D_K / kHz	**0.313**	0.615	-0.027	-0.048	-0.014	-0.103	-0.060	-0.072	-0.013	0.295	0.294	0.455
d_1 / kHz	**-0.010**	-0.026	-0.007	-0.011	-0.018	-0.013	-0.009	-0.018	-0.010	-0.013	-0.012	-0.020
d_2 / kHz	**0.000**	0.000	-0.001	-0.001	0.001	-0.002	-0.003	-0.005	0.005	-0.000	0.002	0.002
$\lvert\mu_a\rvert$ / D	**2.2**	2.1	0.6	1.0	1.4	1.0	1.7	1.6	1.7	1.8	1.8	1.9
$\lvert\mu_b\rvert$ / D	**2.6**	3.5	2.6	1.9	2.3	3.1	3.0	2.3	2.7	2.3	2.1	2.4
$\lvert\mu_c\rvert$ / D	**0.4**	0.6	1.9	1.1	0.2	1.1	1.2	0.5	0.7	0.6	1.4	0.1
ΔE / kJ mol^{-1} [b]	**1.9**	1.0	0.0	0.8	4.2	4.6	2.4	4.2	6.6	1.6	4.0	8.5
ΔG / kJ mol^{-1}	**0.4**	0.0	0.9	0.1	3.1	3.5	2.1	2.4	2.9	0.3	2.9	7.2
E_B / kJ mol^{-1}	**-46.9**	-46.5	-46.2	-47.4	-46.7	-44.3	-47.1	-47.7	-43.5	-45.4	-45.6	-44.6
ΔE_B / kJ mol^{-1}	**0.8**	1.2	1.5	0.3	1.0	3.4	0.6	0.0	4.2	2.3	2.1	3.1

[a]Rotational constants (A, B, C), 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). [b]Relative energies corrected with the zero-point energy (ΔE), Gibbs energy (ΔG, 298K, 1 atm) and complexation energy including BSSE corrections (ΔE_B) relative to the monomers in the geometry of the dimer.

Table S8. Conformational search and predicted rotational parameters for the dimer (thenyl alcohol)$_2$ using B2PLYP-D3(BJ)/def2-TZVP. The isomers observed experimentally are marked in bold characters.

	Isomers											
	O-H···O-H···π				O-H···O-H···π				O-H···O, π···π			
	G´G´-GG´-Lp+	**G´G´-G´G´-Lp+**	G´G´-GG-Lp-	G´G´-G´G-Lp-	A´G-GG´-Lp+	A´G-G´G´-Lp+	A´G-GG-Lp-	A´G-G´G-Lp-	GG´-G´G´-Lp-	G´G´-G´G´-Lp-	G´G´-AG´-Lp-	GG´-AG´-Lp-
A / MHz[a]	**859.03**	**829.55**	760.80	750.23	748.09	750.05	723.30	733.43	833.39	887.25	891.30	841.52
B / MHz	**358.74**	**393.18**	452.27	457.79	440.93	446.95	464.85	449.85	412.58	377.62	384.05	408.81
C / MHz	**329.32**	**357.42**	392.85	402.58	385.79	388.88	397.48	388.93	353.01	325.88	342.22	355.30
D_J / kHz	**0.517**	**0.241**	0.118	0.074	0.125	0.105	0.083	0.144	0.211	0.905	0.197	0.116
D_{JK} / kHz	**-1.612**	**0.912**	-1.298	-0.038	-0.079	-0.118	-0.143	-0.059	-0.290	-2.777	0.085	0.321
D_K / kHz	**1.312**	**-0.712**	1.267	0.096	0.136	0.154	0.132	0.185	0.490	2.336	0.008	-0.123
d_1 / kHz	**-0.128**	**-0.045**	0.013	-0.011	-0.031	-0.013	-0.014	-0.048	-0.005	0.019	-0.003	-0.019
d_2 / kHz	**-0.005**	**-0.003**	-0.006	-0.001	-0.002	-0.002	-0.005	-0.017	0.010	-0.019	0.000	0.002
$\lvert\mu_a\rvert$ / D	**2.1**	**2.1**	1.4	0.94	1.5	1.1	1.6	1.8	1.7	1.5	1.7	1.8
$\lvert\mu_b\rvert$ / D	**2.6**	**3.7**	2.5	1.88	2.3	3.1	3.1	2.3	2.7	2.5	2.1	2.4
$\lvert\mu_c\rvert$ / D	**0.4**	**0.1**	2.1	1.11	0.2	1.1	1.3	0.4	0.7	0.7	1.5	0.0
ΔE / kJ mol^{-1} [b]	**1.6**	**0.4**	0.1	0.0	3.8	4.3	1.9	3.6	6.4	1.8	3.7	8.2
ΔG / kJ mol^{-1}	**0.0**	**1.1**	1.1	2.9	4.4	6.2	4.6	2.9	5.2	8.6	4.3	9.8
E_B / kJ mol^{-1}	**-41.8**	**-40.8**	-41.3	-42.9	-41.3	-39.4	-42.5	-42.9	-38.5	-39.2	-40.3	-39.6
ΔE_B / kJ mol^{-1}	**1.1**	**2.1**	1.6	0.0	1.6	3.5	0.4	0.0	4.4	3.7	2.6	3.3

[a]Rotational constants (A, B, C), 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). [b]Relative energies corrected with the zero-point energy (ΔE), Gibbs energy (ΔG, 298K, 1 atm) and complexation energy including BSSE corrections (ΔE_B) relative to the monomers in the geometry of the dimer.

Table S9. Observed rotational transitions of isomer 1 of the furfuryl alcohol dimer (*Freq.*) and residuals (*o.-c.*) corresponding to the fit of Table 1 (all values in MHz).

J	K_{-1}	K_{+1}	*J*	K_{-1}	K_{+1}	*Freq.*	*o.-c.*
5	2	4	5	1	5	2007.9125	0.0031
6	2	5	6	1	6	2059.2250	-0.0048
8	2	7	8	1	8	2188.4751	0.0053
9	2	8	9	1	9	2266.5127	-0.0106
2	1	2	1	0	1	2312.7877	0.0036
10	2	9	10	1	10	2353.5627	-0.0092
2	1	1	1	0	1	2363.0502	0.0018
11	2	10	11	1	11	2449.5878	-0.0041
5	1	4	4	2	3	2519.7628	0.0036
3	1	3	2	1	2	2541.0379	-0.0132
12	2	11	12	1	12	2554.5004	-0.0059
3	0	3	2	0	2	2565.0379	-0.0037
3	2	2	2	2	1	2566.4004	-0.0019
3	2	1	2	2	0	2567.7379	-0.0064
3	1	2	2	1	1	2591.3129	0.0072
13	2	12	13	1	13	2668.1754	-0.0029
4	0	4	3	1	2	2739.7505	-0.0043
14	3	11	14	2	12	2822.4880	-0.0170
4	0	4	3	1	3	2840.2755	0.0019
7	2	6	6	3	3	2843.8630	-0.0097
13	3	10	13	2	11	2884.2256	-0.0014
7	2	5	6	3	3	2885.5006	-0.0064
7	2	5	6	3	4	2885.8631	0.0036
12	3	9	12	2	10	2940.0256	0.0002
11	3	9	11	2	9	2976.2631	0.0220
11	3	8	11	2	9	2988.6256	-0.0077
10	3	8	10	2	8	3022.2382	-0.0073
10	3	7	10	2	8	3029.3632	-0.0023
9	3	7	9	2	7	3058.2382	-0.0217
6	1	6	5	2	3	3060.2257	-0.0002
9	3	6	9	2	7	3062.1132	0.0034
8	3	6	8	2	6	3085.3507	0.0172
8	3	5	8	2	6	3087.2632	-0.0011
7	3	5	7	2	5	3104.7507	0.0034
7	3	4	7	2	5	3105.6257	-0.0012
6	3	4	6	2	4	3117.8882	-0.0152
6	3	3	6	2	4	3118.2632	0.0072
5	3	3	5	2	3	3126.1882	-0.0225
5	3	2	5	2	3	3126.3382	0.0098
4	3	1	4	2	2	3131.0132	-0.0024
4	3	2	4	2	3	3136.0007	-0.0114
5	3	3	5	2	4	3137.9007	-0.0061

6	3	4	6	2	5	3141.2007	0.0085
6	3	3	6	2	5	3141.5507	0.0060
3	1	3	2	0	2	3143.2507	0.0109
7	3	5	7	2	6	3146.3757	-0.0058
7	3	4	7	2	6	3147.2632	0.0019
8	3	6	8	2	7	3154.0258	-0.0173
8	3	5	8	2	7	3155.9883	0.0142
9	3	7	9	2	8	3164.7883	0.0015
9	3	6	9	2	8	3168.6008	-0.0358
10	3	8	10	2	9	3179.2633	0.0138
11	3	9	11	2	10	3198.1008	0.0197
12	3	10	12	2	11	3221.9383	0.0085
3	1	2	2	0	2	3243.7633	0.0048
13	3	11	13	2	12	3251.4383	0.0107
4	1	4	3	1	3	3387.6634	-0.0024
6	1	5	5	2	3	3411.6009	-0.0051
4	0	4	3	0	3	3418.4634	-0.0082
4	2	3	3	2	2	3421.5759	-0.0079
4	3	1	3	3	0	3422.5259	-0.0345
6	1	5	5	2	4	3423.3009	-0.0012
4	2	2	3	2	1	3424.9259	-0.0062
4	1	3	3	1	2	3454.6259	-0.0176
5	0	5	4	1	3	3555.6635	-0.0122
2	2	1	1	1	0	3583.4885	-0.0039
2	2	0	1	1	0	3583.8135	-0.0147
2	2	1	1	1	1	3600.2510	0.0031
2	2	0	1	1	1	3600.5885	0.0048
5	0	5	4	1	4	3723.1886	0.0164
4	1	4	3	0	3	3965.8638	-0.0001
4	1	3	3	0	3	4133.3639	0.0034
10	3	8	9	4	5	4175.8014	0.0157
10	3	7	9	4	6	4182.9264	-0.0352
5	1	5	4	1	4	4233.9515	0.0030
5	0	5	4	0	4	4270.5640	-0.0004
5	2	4	4	2	3	4276.5265	0.0059
5	4	1	4	4	0	4278.1015	-0.0049
5	3	3	4	3	2	4278.4515	0.0361
5	3	2	4	3	1	4278.4515	-0.0520
5	2	3	4	2	2	4283.2140	0.0232
7	1	6	6	2	4	4310.7515	-0.0229
5	1	4	4	1	3	4317.6140	0.0141
14	4	10	14	3	11	4328.7515	-0.0001
7	1	6	6	2	5	4334.0640	0.0008
11	4	7	11	3	8	4368.5890	-0.0221
10	4	6	10	3	7	4375.4640	-0.0063
13	4	10	13	3	11	4377.5140	-0.0165
12	4	9	12	3	10	4379.0140	0.0070
9	4	5	9	3	6	4380.2640	0.0035

11	4	8	11	3	9	4380.7140	-0.0110
10	4	7	10	3	8	4382.4516	-0.0084
8	4	4	8	3	5	4383.5016	0.0004
9	4	6	9	3	7	4384.0641	0.0097
7	4	4	7	3	5	4386.4391	-0.0435
3	2	2	2	1	1	4422.2016	-0.0044
3	2	1	2	1	1	4423.8766	-0.0071
3	2	2	2	1	2	4472.4641	-0.0062
3	2	1	2	1	2	4474.1516	0.0036
8	1	8	7	2	5	4609.1392	-0.0146
6	0	6	5	1	5	4610.2517	-0.0013
5	1	5	4	0	4	4781.3393	-0.0014
5	1	4	4	0	4	5032.5020	0.0133
11	3	9	10	4	6	5033.9020	0.0028
6	1	6	5	1	5	5079.8395	0.0082
6	0	6	5	0	5	5121.0270	-0.0022
6	2	5	5	2	4	5131.1520	0.0002
6	4	2	5	4	1	5133.9145	-0.0009
6	3	4	5	3	3	5134.4395	0.0024
6	3	3	5	3	2	5134.6770	0.0050
6	2	4	5	2	3	5142.7520	0.0076
7	0	7	6	1	5	5148.6770	0.0063
6	1	5	5	1	4	5180.0771	0.0135
8	1	7	7	2	5	5210.0021	-0.0230
8	1	7	7	2	6	5251.6521	-0.0073
4	2	3	3	1	2	5252.4771	-0.0071
4	2	2	3	1	2	5257.5021	-0.0080
4	2	3	3	1	3	5353.0147	0.0116
9	1	9	8	2	6	5357.3647	-0.0175
4	2	2	3	1	3	5358.0272	-0.0017
10	2	9	9	3	6	5376.7897	-0.0070
7	0	7	6	1	6	5500.0523	0.0015
10	2	8	9	3	7	5537.6648	0.0143
6	1	6	5	0	5	5590.6148	0.0072
12	5	7	12	4	8	5634.1774	-0.0029
11	5	6	11	4	7	5636.5899	0.0184
11	5	7	11	4	8	5636.8774	0.0306
10	5	5	10	4	6	5638.3649	0.0109
10	5	6	10	4	7	5638.5024	0.0193
9	5	4	9	4	5	5639.6524	0.0033
9	5	5	9	4	6	5639.6524	-0.0522
8	5	4	8	4	5	5640.5649	-0.0152
7	5	2	7	4	3	5641.1774	0.0086
6	5	1	6	4	2	5641.5524	0.0003
5	5	1	5	4	2	5641.7649	-0.0056
3	3	1	2	2	0	5701.1149	-0.0125
3	3	0	2	2	1	5701.4649	-0.0024
8	0	8	7	1	6	5922.9526	-0.0145

7	1	7	6	1	6	5925.2526	-0.0042
6	1	5	5	0	5	5941.9776	-0.0100
7	0	7	6	0	6	5969.6276	-0.0015
7	2	6	6	2	5	5985.4401	0.0227
7	5	3	6	5	2	5989.4401	-0.0043
7	3	5	6	3	4	5990.6026	-0.0041
7	3	4	6	3	3	5991.1276	-0.0063
7	2	5	6	2	4	6003.7776	0.0146
7	1	6	6	1	5	6041.9151	0.0022
5	2	4	4	1	3	6074.3652	0.0039
10	1	10	9	2	7	6085.3152	-0.0193
5	2	3	4	1	3	6086.0527	-0.0046
9	1	8	8	2	7	6175.6152	-0.0036
11	2	10	10	3	7	6211.3027	0.0142
5	2	4	4	1	4	6241.8653	0.0075
5	2	3	4	1	4	6253.5528	-0.0010
8	0	8	7	1	7	6391.0029	-0.0004
7	1	7	6	0	6	6394.8404	0.0052
11	2	9	10	3	8	6440.2529	0.0043
4	3	2	3	2	1	6555.9030	-0.0153
4	3	1	3	2	2	6557.6530	0.0275
9	0	9	8	1	7	6680.6780	0.0001
8	1	8	7	1	7	6770.1781	-0.0003
8	0	8	7	0	7	6816.2156	0.0062
8	2	7	7	2	6	6839.2532	-0.0046
8	5	4	7	5	3	6845.2532	0.0016
8	4	4	7	4	3	6845.8532	-0.0085
8	3	6	7	3	5	6846.9282	0.0086
8	3	5	7	3	4	6847.9782	0.0074
7	1	6	6	0	6	6862.8782	0.0069
8	2	6	7	2	5	6866.3532	0.0198
6	2	5	5	1	4	6887.9157	0.0024
13	6	8	13	5	9	6890.7907	-0.0038
12	6	7	12	5	8	6892.1782	0.0054
11	6	5	11	5	6	6893.2282	0.0040
10	6	5	10	5	6	6894.0032	-0.0068
9	6	3	9	5	4	6894.5657	-0.0024
8	6	2	8	5	4	6894.9407	-0.0057
7	6	2	7	5	3	6895.1782	-0.0047
6	6	0	6	5	2	6895.3282	0.0149
8	1	7	7	1	6	6903.0157	0.0020
6	2	4	5	1	4	6911.2157	0.0138
10	1	9	9	2	7	6998.8408	0.0041
12	2	11	11	3	8	7038.7783	0.0136
10	1	9	9	2	8	7105.3158	-0.0477
6	2	5	5	1	5	7139.0533	-0.0078
6	2	4	5	1	5	7162.3659	0.0161
8	1	8	7	0	7	7195.4034	0.0189

9	0	9	8	1	8	7281.5659	0.0167
5	3	3	4	2	2	7409.4035	0.0019
5	3	2	4	2	2	7409.5410	0.0218
5	3	3	4	2	3	7414.3785	-0.0489
5	3	2	4	2	3	7414.5660	0.0209
9	0	9	8	0	8	7660.7287	0.0043
9	2	8	8	2	7	7692.6037	-0.0116
7	2	6	6	1	5	7693.2787	0.0116
9	5	4	8	5	3	7701.1287	0.0010
9	4	5	8	4	4	7702.0287	-0.0085
9	2	7	8	2	6	7730.4412	0.0087
7	2	5	6	1	5	7734.9037	0.0024
9	1	8	8	1	7	7763.2163	-0.0009
8	1	7	7	0	7	7796.2663	0.0105
4	4	0	3	3	1	7810.6288	-0.0057
9	1	9	8	0	8	7993.7539	0.0170

Table S10. Observed rotational transitions of isomer 2 of the furfuryl alcohol dimer (*Freq.*) and residuals (*o.-c.*) corresponding to the fit of Table 1 (all values in MHz).

J	K_{-1}	K_{+1}	J	K_{-1}	K_{+1}	*Freq.*	*o.-c.*
5	2	3	5	1	5	2176.5501	-0.0027
6	2	4	6	1	6	2225.0251	-0.0143
7	2	5	7	1	7	2284.7877	0.0057
2	1	1	1	0	1	2340.1002	0.0136
6	1	5	5	2	3	2958.7756	-0.0112
8	2	6	7	3	4	3110.2757	0.0059
3	1	2	2	0	2	3175.9383	-0.0088
5	0	5	4	1	3	3313.4884	0.0072
11	3	9	11	2	9	3345.6634	0.0139
10	3	8	10	2	8	3375.0259	-0.0660
9	3	7	9	2	7	3397.7134	0.0073
8	3	6	8	2	6	3414.4509	0.0082
7	3	5	7	2	5	3426.3009	0.0014
6	3	4	6	2	4	3434.2634	0.0000
5	3	3	5	2	3	3439.2509	-0.0101
4	3	2	4	2	2	3442.1259	0.0043
3	3	1	3	2	1	3443.5634	0.0112
3	3	0	3	2	2	3444.5634	0.0033
4	3	1	4	2	3	3445.1509	0.0001
5	3	2	5	2	4	3446.3384	-0.0036
6	3	3	6	2	5	3448.4384	-0.0080
7	3	4	7	2	6	3451.8634	0.0141
8	3	5	8	2	7	3457.0259	0.0114
9	3	6	9	2	8	3464.5010	0.0095
10	3	7	10	2	9	3474.9385	0.0168
11	3	8	11	2	10	3489.0593	0.0128
12	3	9	12	2	11	3507.7135	-0.0015
13	3	10	13	2	12	3531.8760	-0.0148
14	3	11	14	2	13	3562.6510	-0.0061
2	2	0	1	1	0	3690.8636	-0.0151
2	2	1	1	1	1	3704.2636	-0.0128
7	1	6	6	2	4	3812.8512	0.0126
9	2	8	8	3	6	3878.3387	-0.0067
9	2	7	8	3	5	3942.5388	-0.0196
4	1	3	3	0	3	4018.9270	0.0057
6	0	6	5	1	4	4088.6895	-0.0147
8	1	8	7	2	6	4204.9896	0.0089
3	2	1	2	1	1	4493.4897	0.0101
3	2	2	2	1	2	4533.2647	-0.0064
8	1	7	7	2	5	4668.6898	0.0011
10	4	7	10	3	7	4814.7649	0.0001
9	4	6	9	3	6	4817.4024	0.0086
10	4	6	10	3	8	4817.9899	0.0041

8	4	5	8	3	5	4819.1649	-0.0165
8	4	4	8	3	6	4820.0399	-0.0066
7	4	4	7	3	4	4820.3524	0.0014
7	4	3	7	3	5	4820.7399	-0.0038
6	4	3	6	3	3	4821.0649	-0.0132
6	4	2	6	3	4	4821.2524	0.0174
5	4	2	5	3	2	4821.5149	0.0158
5	4	1	5	3	3	4821.5649	0.0135
4	4	0	4	3	2	4821.7149	-0.0160
7	0	7	6	1	5	4853.7252	0.0024
5	1	4	4	0	4	4869.3834	-0.0142
9	1	9	8	2	7	4956.0149	-0.0036
4	2	2	3	1	2	5290.4401	-0.0074
4	2	3	3	1	3	5369.0151	-0.0119
9	1	8	8	2	6	5524.8027	0.0028
8	0	8	7	1	6	5607.5777	0.0011
6	1	5	5	0	5	5727.9153	0.0140
3	3	0	2	2	0	5890.5404	-0.0003
3	3	1	2	2	1	5890.7404	0.0002
5	2	3	4	1	3	6082.6030	0.0074
12	5	8	12	4	8	6194.9280	-0.0154
12	5	7	12	4	9	6195.1405	0.0120
10	5	6	10	4	6	6197.3030	-0.0206
10	5	5	10	4	7	6197.4155	0.0488
9	5	4	9	4	6	6198.0780	-0.0004
8	5	3	8	4	5	6198.5780	-0.0020
7	5	2	7	4	4	6198.9030	-0.0110
6	5	1	6	4	3	6199.1030	-0.0160
5	5	1	5	4	1	6199.2280	-0.0016
5	2	4	4	1	4	6211.5530	-0.0017
9	0	9	8	1	7	6349.2906	0.0107
10	1	9	9	2	7	6379.4906	0.0016
7	1	6	6	0	6	6595.0782	0.0001
4	3	1	3	2	1	6705.5533	0.0074
4	3	2	3	2	2	6706.5408	0.0019
6	2	4	5	1	4	6870.9534	0.0096
6	2	5	5	1	5	7060.8909	0.0145
10	0	10	9	1	8	7077.8763	-0.0060
11	1	10	10	2	8	7230.9785	0.0052
8	1	7	7	0	7	7471.6640	-0.0076
5	3	2	4	2	2	7519.8037	0.0074
5	3	3	4	2	3	7522.7537	-0.0066
7	2	5	6	1	5	7656.7037	-0.0020
7	2	6	6	1	6	7917.0164	-0.0061

Table S11. Observed rotational transitions of isomer 1 of the thenyl alcohol dimer (*Freq.*) and residuals (*o.-c.*) corresponding to the fit of Table 2 (all values in MHz).

J	K_{-1}	K_{+1}	*J*	K_{-1}	K_{+1}	*Freq.*	*o.-c.*
3	1	3	2	1	2	2139.3750	0.0085
3	0	3	2	0	2	2184.6250	-0.0099
3	2	2	2	2	1	2192.4125	0.0096
3	2	1	2	2	0	2200.1625	-0.0050
6	3	3	6	2	4	2205.1250	-0.0100
3	1	2	2	1	1	2242.9750	-0.0164
5	3	2	5	2	3	2245.9500	0.0095
4	3	1	4	2	2	2271.4000	-0.0093
4	3	2	4	2	3	2299.7875	-0.0040
8	3	6	8	2	7	2394.2375	-0.0103
4	0	4	3	1	3	2540.5125	-0.0117
3	1	3	2	0	2	2548.1375	-0.0108
2	2	1	1	1	0	2820.3500	-0.0020
4	1	4	3	1	3	2850.3625	0.0063
2	2	0	1	1	1	2856.8625	-0.0060
4	0	4	3	0	3	2904.0250	-0.0125
4	2	3	3	2	2	2921.6750	0.0021
4	3	1	3	3	0	2927.3000	-0.0141
4	2	2	3	2	1	2940.8375	0.0166
4	1	3	3	1	2	2988.2000	0.0000
10	4	6	10	3	7	3098.5875	0.0069
7	4	3	7	3	4	3187.0125	0.0089
5	4	2	5	3	3	3205.6750	0.0030
4	1	4	3	0	3	3213.8750	0.0055
5	0	5	4	1	4	3306.8625	0.0067
3	2	2	2	1	1	3516.5875	0.0021
5	1	5	4	1	4	3559.7250	0.0113
5	0	5	4	0	4	3616.7000	0.0123
3	2	1	2	1	2	3630.0000	0.0035
5	2	4	4	2	3	3649.6250	-0.0103
5	3	3	4	3	2	3659.9875	-0.0010
5	3	2	4	3	1	3661.4250	-0.0029
5	2	3	4	2	2	3686.9000	0.0031
5	1	4	4	1	3	3731.1000	0.0068
5	1	5	4	0	4	3869.5500	0.0044
6	0	6	5	1	5	4069.5250	0.0056
7	1	6	6	2	5	4175.6500	-0.0091
4	2	3	3	1	2	4195.2625	-0.0043
6	1	6	5	1	5	4267.2625	0.0039
6	0	6	5	0	5	4322.3750	-0.0022
6	2	5	5	2	4	4375.9750	-0.0001
6	3	4	5	3	3	4393.6375	-0.0051

6	3	3	5	3	2	4397.4500	-0.0002
4	2	2	3	1	3	4431.4375	-0.0133
6	2	4	5	2	3	4438.2500	-0.0057
6	1	5	5	1	4	4470.8250	-0.0045
3	3	1	2	2	0	4485.0250	0.0103
3	3	0	2	2	1	4487.0250	-0.0101
6	1	6	5	0	5	4520.1250	0.0086
7	0	7	6	1	6	4824.3375	0.0139
5	2	4	4	1	3	4856.7000	-0.0020
7	1	7	6	1	6	4972.9375	0.0061
7	0	7	6	0	6	5022.0625	-0.0002
7	2	6	6	2	5	5100.3875	-0.0063
7	5	2	6	5	1	5122.4750	0.0121
7	4	4	6	4	3	5125.1250	-0.0054
7	4	3	6	4	2	5125.3625	-0.0088
7	3	5	6	3	4	5127.6625	-0.0108
7	3	4	6	3	3	5136.1250	-0.0006
7	1	7	6	0	6	5170.6750	0.0045
7	2	5	6	2	4	5193.5625	-0.0077
7	1	6	6	1	5	5206.4250	0.0112
4	3	2	3	2	1	5211.7500	0.0018
4	3	1	3	2	2	5221.9500	0.0035
5	2	3	4	1	4	5268.0000	0.0084
6	2	5	5	1	4	5501.6000	0.0159
10	2	8	9	3	7	5527.2250	0.0133
8	0	8	7	1	7	5568.9500	0.0017
8	1	8	7	1	7	5676.8000	0.0130
8	0	8	7	0	7	5717.5625	0.0064
8	2	7	7	2	6	5822.6125	-0.0084
8	1	8	7	0	7	5825.4000	0.0053
9	1	8	8	2	7	5849.9750	0.0095
8	6	2	7	6	1	5853.6625	0.0056
8	5	3	7	5	2	5855.8250	-0.0035
8	4	5	7	4	4	5859.6875	0.0058
8	4	4	7	4	3	5860.3250	-0.0148
8	3	6	7	3	5	5861.7750	-0.0021
8	3	5	7	3	4	5878.3250	-0.0005
5	3	3	4	2	2	5930.9125	-0.0033
8	1	7	7	1	6	5936.7125	-0.0081
8	2	6	7	2	5	5950.6250	0.0068
5	3	2	4	2	3	5961.7000	-0.0016
7	2	6	6	1	5	6131.1375	-0.0109
4	4	1	3	3	0	6134.1750	0.0038
6	2	4	5	1	5	6146.5375	0.0038
9	0	9	8	1	8	6303.0125	0.0204
9	1	9	8	1	8	6378.9750	0.0019
9	0	9	8	0	8	6410.8250	-0.0056
9	1	9	8	0	8	6486.8125	0.0008

9	2	8	8	2	7	6542.3625	-0.0652
9	7	3	8	7	1	6584.9000	-0.0147
9	7	3	8	7	2	6584.9125	-0.0022
9	6	3	8	6	2	6586.7250	0.0006
9	5	5	8	5	4	6589.8250	0.0225
9	5	4	8	5	3	6589.8250	-0.0154
9	4	6	8	4	5	6595.0500	0.0022
9	3	7	8	3	6	6595.5625	0.0036
9	4	5	8	4	4	6596.6125	-0.0005
9	3	6	8	3	5	6624.9375	-0.0034
6	3	4	5	2	3	6637.6625	0.0009
9	1	8	8	1	7	6660.6000	-0.0004
10	1	9	9	2	8	6684.6250	-0.0142
9	2	7	8	2	6	6706.9500	-0.0040
6	3	3	5	2	4	6709.5125	-0.0040
8	2	7	7	1	6	6747.3625	0.0068
5	4	2	4	3	1	6865.1750	-0.0034
5	4	1	4	3	2	6865.6500	-0.0286
10	0	10	9	1	9	7027.4375	-0.0018
7	2	5	6	1	6	7072.8625	0.0172
10	1	10	9	1	9	7079.7000	-0.0001
10	0	10	9	0	9	7103.4250	0.0046
10	1	10	9	0	9	7155.6625	-0.0186
10	2	9	9	2	8	7259.6500	0.0061
10	8	3	9	8	2	7316.2125	0.0094
10	7	4	9	7	3	7317.7750	-0.0058
10	6	4	9	6	3	7320.2750	0.0001
10	3	8	9	3	7	7328.5625	-0.0015
10	4	7	9	4	6	7331.2000	0.0025
10	4	6	9	4	5	7334.5500	0.0042
9	2	8	8	1	7	7353.0625	-0.0002
10	3	7	9	3	6	7376.6625	0.0072
10	1	9	9	1	8	7377.1000	-0.0015
10	2	8	9	2	7	7460.4875	0.0031
7	3	4	6	2	5	7469.6750	0.0079
11	1	10	10	2	9	7510.7875	-0.0089
6	4	3	5	3	2	7595.1000	-0.0174
6	4	2	5	3	3	7597.1375	0.0078
11	0	11	10	1	10	7743.9750	0.0196
11	1	11	10	1	10	7779.2125	0.0038
5	5	0	4	4	1	7782.3375	0.0085
11	0	11	10	0	10	7796.2125	-0.0036
11	1	11	10	0	10	7831.4625	-0.0069
11	2	10	10	2	9	7974.1625	-0.0088
8	3	6	7	2	5	7995.3125	0.0264
11	3	9	10	3	8	8060.3125	-0.0032
11	4	7	10	4	6	8074.6125	0.0070
11	3	8	10	3	7	8133.6125	0.0056

Table S12. Observed rotational transitions of isomer 2 of the thenyl alcohol dimer (Freq.) and residuals (*o.-c.*) corresponding to the fit of Table 2 (all values in MHz).

J	K_{-1}	K_{+1}	*J*	K_{-1}	K_{+1}	*Freq.*	*o-c*
10	1	9	10	0	10	2060.8000	-0.0046
8	2	7	8	1	8	2071.0500	0.0075
6	3	3	6	2	4	2075.5625	0.0106
5	3	2	5	2	3	2129.0750	-0.0007
3	1	3	2	1	2	2185.6875	-0.0064
4	3	2	4	2	3	2203.0750	-0.0010
5	3	3	5	2	4	2217.4375	-0.0024
3	0	3	2	0	2	2236.6000	0.0000
6	3	4	6	2	5	2241.7500	-0.0131
3	2	2	2	2	1	2247.4875	-0.0083
3	2	1	2	2	0	2258.3750	-0.0071
9	2	8	9	1	9	2259.6375	-0.0051
6	2	5	5	3	2	2261.8750	-0.0009
7	3	5	7	2	6	2278.9875	0.0027
3	1	2	2	1	1	2305.8250	-0.0222
8	3	6	8	2	7	2331.8750	0.0017
11	1	10	11	0	11	2375.5125	0.0125
9	3	7	9	2	8	2402.8250	-0.0105
6	2	4	5	3	3	2441.0750	0.0091
10	2	9	10	1	10	2465.8250	0.0122
14	4	10	14	3	11	2473.8250	-0.0101
10	3	8	10	2	9	2493.7625	-0.0008
3	1	3	2	0	2	2567.1375	0.0099
13	4	9	13	3	10	2597.5750	0.0038
11	3	9	11	2	10	2605.9125	-0.0050
6	1	6	5	2	3	2637.5125	-0.0073
4	0	4	3	1	3	2639.4250	0.0081
11	2	10	11	1	11	2687.3500	0.0049
5	1	4	4	2	3	2711.1500	-0.0222
12	4	8	12	3	9	2716.5875	0.0092
12	3	10	12	2	11	2739.8500	-0.0056
2	2	1	1	1	0	2794.7625	0.0002
11	4	7	11	3	8	2820.8000	0.0040
2	2	0	1	1	1	2837.6125	0.0163
13	3	11	13	2	12	2895.4125	0.0069
10	4	6	10	3	7	2904.5375	0.0112
4	1	4	3	1	3	2911.3000	-0.0042
12	2	11	12	1	12	2921.8500	0.0147
8	3	6	7	4	3	2952.5250	0.0065
9	4	5	9	3	6	2966.5750	-0.0008
4	0	4	3	0	3	2969.9250	-0.0195
7	2	6	6	3	3	2971.3125	-0.0248

4	2	3	3	2	2	2994.5000	-0.0067
13	1	12	13	0	13	3001.4875	0.0237
4	3	2	3	3	1	3001.7875	-0.0204
4	3	1	3	3	0	3002.5125	0.0011
8	3	5	7	4	4	3004.6375	-0.0064
8	4	4	8	3	5	3009.2125	0.0057
4	2	2	3	2	1	3021.1750	-0.0124
7	4	3	7	3	4	3036.4875	0.0155
6	4	2	6	3	3	3052.7125	-0.0088
8	4	5	8	3	6	3058.6125	-0.0023
7	4	4	7	3	5	3059.7000	-0.0104
9	4	6	9	3	7	3060.8500	0.0013
6	4	3	6	3	4	3062.2375	-0.0082
10	4	7	10	3	8	3068.8250	-0.0161
4	1	3	3	1	2	3070.9750	0.0161
14	3	12	14	2	13	3071.7000	0.0091
11	4	8	11	3	9	3085.4125	-0.0049
12	4	9	12	3	10	3113.5875	-0.0095
7	1	7	6	2	4	3145.0250	-0.0097
13	4	10	13	3	11	3156.3625	-0.0027
14	4	11	14	3	12	3216.4500	0.0024
4	1	4	3	0	3	3241.8250	-0.0068
15	3	13	15	2	14	3267.2125	0.0008
7	2	5	6	3	4	3280.3250	-0.0055
15	4	12	15	3	13	3296.1125	0.0001
14	1	13	14	0	14	3305.1250	-0.0037
16	4	13	16	3	14	3397.0125	-0.0031
14	2	13	14	1	14	3420.1500	-0.0022
5	0	5	4	1	4	3422.5125	-0.0019
3	2	2	2	1	1	3503.8375	0.0026
6	1	5	5	2	4	3561.3000	-0.0066
5	1	5	4	1	4	3634.7000	-0.0110
3	2	1	2	1	2	3637.7375	0.0008
5	0	5	4	0	4	3694.3875	-0.0142
5	2	4	4	2	3	3739.6875	0.0067
5	4	2	4	4	1	3751.9375	0.0242
5	4	1	4	4	0	3751.9375	-0.0091
5	3	3	4	3	2	3754.0500	0.0054
5	3	2	4	3	1	3756.4750	-0.0155
5	2	3	4	2	2	3791.0000	-0.0021
13	5	8	13	4	9	3803.9625	-0.0061
9	3	6	8	4	5	3805.8125	0.0045
5	1	4	4	1	3	3832.7000	-0.0077
12	5	7	12	4	8	3850.4625	0.0164
15	5	11	15	4	12	3881.1625	0.0035
14	5	10	14	4	11	3881.9250	-0.0076
11	5	6	11	4	7	3883.0125	0.0156
13	5	9	13	4	10	3888.0625	0.0031

16	5	12	16	4	13	3888.5500	0.0051
12	5	8	12	4	9	3897.1250	-0.0006
10	5	5	10	4	6	3905.3375	0.0062
5	1	5	4	0	4	3906.5875	-0.0108
11	5	7	11	4	8	3907.2125	-0.0063
10	5	6	10	4	7	3916.9625	-0.0046
9	5	4	9	4	5	3920.4125	-0.0004
9	5	5	9	4	6	3925.5000	-0.0133
8	5	3	8	4	4	3930.4375	-0.0056
6	5	2	6	4	3	3941.3000	-0.0207
5	5	0	5	4	1	3943.6250	-0.0210
8	2	6	7	3	5	4145.7625	-0.0109
4	2	3	3	1	2	4192.5000	0.0056
6	0	6	5	1	5	4198.2250	-0.0005
9	2	8	8	3	5	4310.6500	0.0112
6	1	6	5	1	5	4355.7375	0.0005
11	4	8	10	5	5	4362.8500	-0.0020
11	4	7	10	5	6	4388.5125	-0.0043
6	0	6	5	0	5	4410.4125	-0.0096
7	1	6	6	2	5	4419.5000	0.0022
3	3	1	2	2	0	4440.5250	-0.0030
3	3	0	2	2	1	4443.4000	0.0116
10	3	8	9	4	5	4449.2750	-0.0207
4	2	2	3	1	3	4473.2250	-0.0051
6	2	5	5	2	4	4482.6000	0.0171
6	5	1	5	5	0	4501.8500	-0.0065
6	4	3	5	4	2	4504.2125	-0.0055
6	4	2	5	4	1	4504.3875	0.0198
6	3	4	5	3	3	4506.9125	0.0064
6	3	3	5	3	2	4513.3500	-0.0007
6	2	4	5	2	3	4566.8625	-0.0121
6	1	6	5	0	5	4567.9375	0.0039
6	1	5	5	1	4	4589.8125	-0.0025
10	3	7	9	4	6	4630.8750	-0.0008
15	6	9	15	5	10	4723.3625	0.0064
15	6	10	15	5	11	4744.7625	-0.0076
14	6	8	14	5	9	4750.2375	0.0074
14	6	9	14	5	10	4761.2875	0.0065
13	6	7	13	5	8	4770.3250	-0.0063
13	6	8	13	5	9	4775.7000	-0.0038
12	6	7	12	5	8	4787.7375	-0.0840
9	6	4	9	5	5	4811.1750	-0.0337
8	6	2	8	5	3	4815.4750	0.0299
8	6	3	8	5	4	4815.4750	-0.0078
7	6	2	7	5	3	4818.4375	-0.0408
6	6	1	6	5	2	4820.4375	-0.0350
5	2	4	4	1	3	4861.2125	-0.0036
10	2	9	9	3	6	4922.1000	-0.0082

7	0	7	6	1	6	4962.5750	-0.0054
9	2	7	8	3	6	5034.5375	-0.0169
7	1	7	6	1	6	5074.4000	0.0104
7	0	7	6	0	6	5120.0875	-0.0043
12	4	8	11	5	7	5179.2750	0.0136
11	3	9	10	4	6	5182.7625	-0.0033
4	3	2	3	2	1	5183.9500	-0.0038
4	3	1	3	2	2	5198.4125	0.0086
7	2	6	6	2	5	5222.8000	-0.0121
7	1	7	6	0	6	5231.9125	0.0115
7	6	2	6	6	1	5251.8375	-0.0075
7	5	2	6	5	1	5253.8375	-0.0090
7	4	4	6	4	3	5257.5125	0.0139
7	4	3	6	4	2	5257.9875	-0.0069
7	3	5	6	3	4	5260.0375	0.0036
7	3	4	6	3	3	5274.2500	0.0062
8	1	7	7	2	6	5280.6500	0.0041
7	1	6	6	1	5	5340.7750	0.0010
7	2	5	6	2	4	5346.1750	0.0042
5	2	3	4	1	4	5352.9375	0.0094
11	2	10	10	3	7	5481.3750	0.0004
11	3	8	10	4	7	5484.6625	-0.0254
6	2	5	5	1	4	5511.1000	0.0086
13	7	7	13	6	8	5671.0750	-0.0571
12	7	5	12	6	6	5678.7875	0.0218
12	7	6	12	6	7	5678.7875	-0.0505
11	7	5	11	6	6	5684.8750	0.0013
10	7	4	10	6	5	5689.5125	0.0157
9	7	3	9	6	4	5692.9625	0.0163
8	7	2	8	6	3	5695.4750	0.0357
7	7	1	7	6	1	5697.1500	-0.0207
7	7	0	7	6	2	5697.1625	-0.0082
8	0	8	7	1	7	5714.3875	0.0003
8	1	8	7	1	7	5790.8500	0.0143
8	0	8	7	0	7	5826.1875	-0.0087
12	3	10	11	4	7	5898.4250	0.0030
8	1	8	7	0	7	5902.6250	-0.0197
5	3	3	4	2	2	5916.8250	0.0140
10	2	8	9	3	7	5942.1375	-0.0125
8	2	7	7	2	6	5960.0250	0.0013
5	3	2	4	2	3	5960.3875	-0.0001
12	2	11	11	3	8	5979.3625	0.0001
13	4	9	12	5	8	5986.5875	-0.0119
8	7	2	7	7	0	6001.8625	-0.0047
8	7	2	7	7	1	6001.8500	-0.0172
8	6	3	7	6	2	6003.6000	0.0012
8	5	3	7	5	2	6006.6125	-0.0111
8	4	5	7	4	4	6011.8125	-0.0039

8	3	6	7	3	5	6012.9125	0.0004
8	4	4	7	4	3	6013.1750	0.0074
8	3	5	7	3	4	6040.4250	-0.0077
4	4	1	3	3	0	6068.8125	0.0569
4	4	0	3	3	1	6068.8125	-0.0648
8	1	7	7	1	6	6083.9500	-0.0103
8	2	6	7	2	5	6125.4750	-0.0017
9	1	8	8	2	7	6138.5625	0.0021
7	2	6	6	1	5	6144.0875	-0.0009
6	2	4	5	1	5	6285.0875	-0.0042
12	3	9	11	4	8	6369.9000	-0.0019
13	2	12	12	3	9	6409.6750	-0.0034
9	0	9	8	1	8	6454.6375	0.0019
9	1	9	8	1	8	6505.3500	-0.0041
9	0	9	8	0	8	6531.0875	0.0034
15	8	8	15	7	9	6544.8250	-0.0110
14	8	7	14	7	8	6552.4125	0.0000
13	8	6	13	7	7	6558.5500	0.0192
12	8	5	12	7	6	6563.4125	0.0184
11	8	4	11	7	5	6567.2000	0.0108
10	8	2	10	7	3	6570.1000	0.0139
9	8	1	9	7	2	6572.2500	0.0111
8	8	1	8	7	1	6573.7750	-0.0110
9	1	9	8	0	8	6581.8125	0.0098
6	3	4	5	2	3	6632.7250	0.0101
9	2	8	8	2	7	6693.9625	0.0081
6	3	3	5	2	4	6734.0625	0.0048
9	8	2	8	8	0	6751.9000	-0.0101
9	7	3	8	7	2	6753.4750	0.0176
9	6	3	8	6	2	6755.9750	0.0230
9	5	5	8	5	4	6760.2125	-0.0120
9	5	4	8	5	3	6760.3000	-0.0193
8	2	7	7	1	6	6763.3500	0.0119
9	3	7	8	3	6	6764.9250	0.0083
9	4	6	8	4	5	6767.1625	0.0119
9	4	5	8	4	4	6770.3500	0.0004
9	3	6	8	3	5	6812.9750	-0.0054
9	1	8	8	1	7	6817.9500	0.0118
5	4	2	4	3	1	6818.1625	0.0051
5	4	1	4	3	2	6819.0125	-0.0034
11	2	9	10	3	8	6863.0250	-0.0101
9	2	7	8	2	6	6901.6875	-0.0054
10	1	9	9	2	8	6986.6000	0.0137
10	0	10	9	1	9	7185.4500	0.0257
10	1	10	9	1	9	7218.2750	-0.0047
10	0	10	9	0	9	7236.1500	0.0072
14	3	12	13	4	9	7243.8250	0.0145
10	1	10	9	0	9	7269.0125	0.0142

7	2	5	6	1	6	7275.5375	0.0119
13	3	10	12	4	9	7286.1625	0.0085
7	3	5	6	2	4	7325.8875	0.0134
9	2	8	8	1	7	7373.3375	0.0054
15	4	12	14	5	9	7410.7125	0.0065
10	2	9	9	2	8	7424.4500	0.0001
16	9	8	16	8	9	7426.0125	-0.0012
15	9	7	15	8	8	7432.1750	-0.0014
14	9	6	14	8	7	7437.2250	0.0091
13	9	4	13	8	5	7441.2875	0.0080
12	9	3	12	8	4	7444.5125	0.0094
11	9	3	11	8	3	7447.0125	0.0016
10	9	2	10	8	2	7448.9125	-0.0040
9	9	1	9	8	1	7450.3250	0.0015
10	9	1	9	9	0	7501.9750	0.0069
10	8	2	9	8	1	7503.3875	0.0125
10	6	4	9	6	3	7508.9875	0.0049
10	5	6	9	5	5	7514.8250	0.0010
10	5	5	9	5	4	7515.0875	0.0003
10	3	8	9	3	7	7515.3750	-0.0027
10	4	7	9	4	6	7523.3750	0.0048
7	3	4	6	2	5	7525.7250	0.0064
10	4	6	9	4	5	7530.1625	-0.0063
10	1	9	9	1	8	7541.9875	0.0072
6	4	3	5	3	2	7565.8875	0.0026
6	4	2	5	3	3	7569.3500	0.0109
10	3	7	9	3	6	7592.2250	0.0065
10	2	8	9	2	7	7672.5125	0.0001
15	4	11	14	5	10	7672.8250	-0.0235
5	5	1	4	4	0	7695.6000	0.0074
5	5	0	4	4	1	7695.6000	0.0031
12	2	10	11	3	9	7790.9500	-0.0112
11	1	10	10	2	9	7818.7625	0.0082
11	1	11	10	1	10	7929.9500	-0.0024
11	0	11	10	0	10	7941.9125	-0.0100
11	1	11	10	0	10	7962.8250	0.0170
10	2	9	9	1	8	7979.8500	0.0061
8	3	6	7	2	5	7992.6250	0.0096
11	2	10	10	2	9	8151.4875	0.0027

Table S13. Equilibrium coordinates for the G´G-G'G-Lp- isomer of (furfuryl alcohol)$_2$, according to the DFT prediction B2PLYP-D3(BJ) /def2TZVP.

Atom	*a* / Å[a]	*b* / Å	*c* / Å
C	-2.6368	0.3518	1.4297
C	-3.6168	0.7950	0.6062
C	-3.1061	0.6721	-0.7254
C	-1.8492	0.1664	-0.6269
O	-1.5466	-0.0319	0.7007
H	-2.5510	0.2476	2.4960
H	-4.5830	1.1610	0.9070
H	-3.6103	0.9223	-1.6429
C	-0.8069	-0.1951	-1.6262
H	-1.1414	0.1692	-2.5969
H	0.1299	0.3171	-1.3843
O	-0.5987	-1.5917	-1.7604
H	-0.1278	-1.8968	-0.9671
C	2.0113	1.9400	0.1673
C	2.7688	1.5093	-0.8742
C	2.8996	0.0950	-0.7122
C	2.2157	-0.2338	0.4171
O	1.6679	0.8943	0.9680
H	1.6492	2.9051	0.4720
H	3.1824	2.1205	-1.6574
H	3.4212	-0.5919	-1.3564
C	1.9057	-1.5146	1.0955
H	2.5761	-2.2858	0.7226
H	2.0607	-1.4154	2.1735
O	0.5785	-1.9826	0.8357
H	-0.0526	-1.3116	1.1368

[a]Principal inertial axes denoted *a*, *b*, *c*.

Table S14. Equilibrium coordinates for the G´G-GG-Lp- isomer of (furfuryl alcohol)$_2$, according to the DFT prediction B2PLYP-D3(BJ) /def2TZVP.

Atom	*a* / Å[a]	*b* / Å	*c* / Å
C	-2.8312	-0.8957	1.0822
C	-3.7706	0.0582	0.8784
C	-3.1597	1.0512	0.0477
C	-1.8885	0.6414	-0.1981
O	-1.6712	-0.5588	0.4410
H	-2.8178	-1.8237	1.6242
H	-4.7739	0.0554	1.2675
H	-3.6094	1.9546	-0.3268
C	-0.7626	1.2060	-0.9916
H	-1.0364	2.2226	-1.2723
H	0.1335	1.2640	-0.3664
O	-0.5006	0.5039	-2.1956
H	-0.0338	-0.3167	-1.9694
C	2.8519	1.4396	0.1190
C	2.5166	1.2996	1.4279
C	2.0355	-0.0384	1.5714
C	2.1128	-0.6162	0.3404
O	2.6154	0.2841	-0.5579
H	3.2551	2.2502	-0.4606
H	2.6037	2.0516	2.1927
H	1.6735	-0.5103	2.4690
C	1.7170	-1.9432	-0.1905
H	2.4647	-2.3050	-0.8946
H	1.6569	-2.6507	0.6400
O	0.4854	-1.9140	-0.9175
H	-0.2252	-1.6791	-0.3016

[a]Principal inertial axes denoted *a*, *b*, *c*.

Table S15. Equilibrium coordinates for the G´G´-G´G´-Lp+ isomer of (thenyl alcohol)$_2$, according to the DFT prediction B2PLYP-D3(BJ) /def2TZVP.

Atom	*a* / Å[a]	*b* / Å	*c* / Å
S	-2.3681	-0.8649	0.5053
C	-2.8955	0.5363	1.3408
C	-2.7730	1.6593	0.5676
C	-2.2396	1.3745	-0.7156
C	-1.9640	0.0438	-0.9036
C	-1.3219	-0.5973	-2.0892
H	-1.8223	-1.5251	-2.3629
H	-1.3931	0.0873	-2.9388
O	0.0412	-0.9630	-1.8560
H	0.5183	-0.1745	-1.5625
H	-2.0567	2.1205	-1.4764
H	-3.0593	2.6452	0.9023
H	-3.2777	0.4585	2.3453
S	3.0584	0.0698	-0.1394
C	2.7051	1.7252	-0.4328
C	1.5411	2.1069	0.1780
C	0.9302	1.0426	0.8926
C	1.6353	-0.1317	0.8206
C	1.2550	-1.4655	1.3857
H	2.0009	-1.8181	2.0995
O	1.1535	-2.4785	0.3993
H	0.6627	-2.1176	-0.3574
H	0.3111	-1.3343	1.9269
H	-0.0071	1.1284	1.4237
H	1.1355	3.1060	0.1160
H	3.3663	2.3228	-1.0385

[a]Principal inertial axes denoted *a*, *b*, *c*.

Table S16. Equilibrium coordinates for the G´G´-GG´-Lp+ isomer of (thenyl alcohol)$_2$, according to the DFT prediction B2PLYP-D3(BJ) /def2TZVP.

Atom	*a* / Å[a]	*b* / Å	*c* / Å
S	-3.2250	-0.0135	0.0632
C	-2.9994	1.6610	0.3688
C	-1.8061	2.1081	-0.1307
C	-1.0677	1.0767	-0.7702
C	-1.7086	-0.1376	-0.7530
C	-1.2038	-1.4412	-1.2912
H	-1.8762	-1.8369	-2.0534
H	-0.2376	-1.2411	-1.7685
O	-1.0967	-2.4530	-0.3036
H	-0.6739	-2.0582	0.4787
H	-0.0959	1.2136	-1.2239
H	-1.4687	3.1304	-0.0437
H	-3.7485	2.2223	0.9025
S	2.5800	1.2371	0.3812
C	3.0625	0.8646	-1.2195
C	2.8420	-0.4565	-1.5124
C	2.2760	-1.1675	-0.4250
C	2.0727	-0.3826	0.6829
C	1.4173	-0.7636	1.9711
H	1.7676	-1.7427	2.2939
O	-0.0034	-0.8932	1.8483
H	-0.3538	-0.0706	1.4772
H	1.6619	-0.0431	2.7560
H	2.0104	-2.2152	-0.4542
H	3.0858	-0.9013	-2.4659
H	3.4971	1.6229	-1.8495

[a]Principal inertial axes denoted *a*, *b*, *c*.

Table S17. Results from a (second-order intramonomer / third-order intermonomer) Symmetry-Adapted Perturbation Theory (SAPT2+(3)/aug-cc-pVDZ) binding energy decomposition of (furfuryl alcohol)$_2$, (thenyl alcohol)$_2$ and related dimers, comparing the magnitude of the attractive contributions (all values in kJ mol^{-1}) See Tables 1-2 for a comparison with the B2PLYP complexation energies.

	$\Delta E_{\text{Electrostatic}}$	$\Delta E_{\text{Induction}}$	$\Delta E_{\text{Dispersion}}$	ΔE_{Exch}	ΔE_{Total}
FA···H_2O – GG´-W_{da}[a]	-57.2 [57.5%] [j]	-20.3 [20.4%]	-22.1[22.2%]	70.5	-29.0
TA···H_2O – GG-Wa[b]	-49.2 [55.5%]	-17.0 [19.2%]	-22.4 [25.3%]	61.7	-26.8
$(FA)_2$ – G´G-G´G- Lp-[c]	-61.7 [49.7%]	-21.5 [17.3%]	-41.0 [33.0%]	85.7	-38.5
$(FA)_2$ – G´G-GG- Lp-[c]	-60.3 [49.1%]	-21.7 [17.7%]	-40.8 [33.2%]	83.9	-39.0
$(TA)_2$ – G´G´-G´G´- Lp+[c]	-51.4 [43.9%]	-16.3 [13.9%]	-49.4 [42.2%]	76.9	-40.3
$(TA)_2$ – G´G´-GG´- Lp+[c]	-57.9 [46.9%]	-18.8[15.2%]	-46.8 [37.9%]	83.0	-40.4
$(Cyclohexanol)_2$ [d]	-46.5 [51.8%]	-16.6 [18.5%]	-26.6 [29.7%]	60.5	-29.2
$(Phenol)_2$ [e]	-41.8 [48.3%]	-28.8 [18.4%]	-15.9 [33.3%]	58.9	-27.6
$(Thiophenol)_2$ [f]	-26.0 [29.4%]	-8.5 [9.6%]	-53.8 [60.9%]	61.3	-30.0
$(H_2O)_2$ [g]	-35.7 [63.5%]	-9.5 [19.8%]	-11.1 [16.8%]	37.7	-18.6
$(H_2S)_2$ [h]	-12.1 [49.0%]	-7.8 [19.3%]	-4.7 [31.7%]	19.2	-5.4
Pyridine - methane [i]	-3.0 [57.5%]	-10.9 [208.1%]	-0.7 [13.5%]	9.4	-5.2

[a]Juanes, M.; Lesarri, A.; Pinacho, R.; Charro, E.; Rubio, J. E.; Enríquez, L.; Jaraíz, *Chem. - A Eur. J.* **2018**, *24* (25), 6564–6571. [b]Juanes, M.; Saragi, R. T.; Pinacho, R.; Rubio, J. E.; Lesarri, A., *Phys. Chem. Chem. Phys.* **2020**, *22* (22), 12412–12421. [c]This work. [d]Juanes, M.; Usabiaga, I.; León, I.; Evangelisti, L.; Fernández, J. A.; Lesarri, A., *Angew. Chemie Int. Ed.* **2020**, *59* (33), 14081–14085. [e]Seifert, N. A.; Steber, A. L.; Neill, J. L.; Pérez, C.; Zaleski, D. P.; Pate, B. H.; Lesarri, A., *Phys. Chem. Chem. Phys.* **2013**, *15* (27), 11468–11477. [f]Saragi, R. T.; Juanes, M.; Pérez, C.; Pinacho, P.; Tikhonov, D. S.; Caminati, W.; Schnell, M.; Lesarri, A., *J. Phys. Chem. Lett.* **2021**, *12* (5), 1367–1373. [g]Dyke, T. R.; Mack, K. M.; Muenter, J. S., *J. Chem. Phys.* **1977**, *66* (2), 498–510. [h]Das, A.; Mandal, P. K.; Lovas, F. J.; Medcraft, C.; Walker, N. R.; Arunan, E., *Angew. Chemie Int. Ed.* **2018**, *57* (46), 15199–15203. [i]Q. Gou, L. Spada, M. Vallejo-López, A. Lesarri, E. J. Cocinero, W. Caminati, Phys. Chem. Chem. Phys., 2014, 16, 13041–13046. [j]Relative percentage of the total attractive interactions for each molecule.