Molecular Recognition, Transient Chirality and Sulfur Hydrogen Bonding in the Benzyl Mercaptan Dimer

SUPPORTING INFORMATION

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Figure S1. Rotational spectrum of benzyl mercaptan in the 3-8 GHz frequency region. The positive trace shows the experimental spectrum; the negative trace is the simulation of fitted rotational constants of the monomer and the dimer (isomer 1, GG-GG-Lp-).
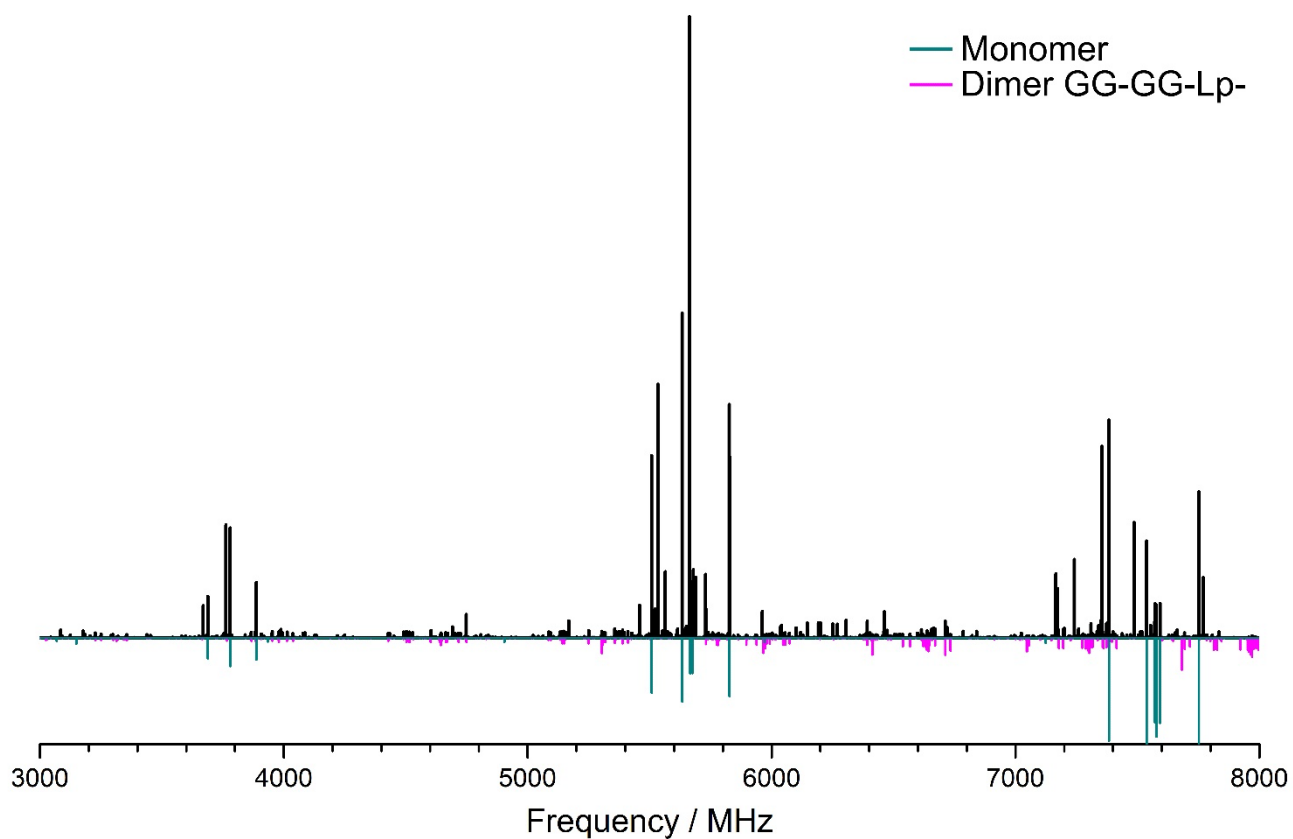
Figure S2. The most stable isomers of the benzyl mercaptan dimer, classified by their intermolecular interactions and ordered by the relative electronic energy (ΔE_{ZPE}, kJ/mol) calculated using B3LYP-D3(BJ)/def2-TZVP. Isomers in the dashed rectangle exhibit a sulfur S-H···S hydrogen bond. The only symmetric isomers are 5 (C_2), 9 (C_2) and 11 (C_i).
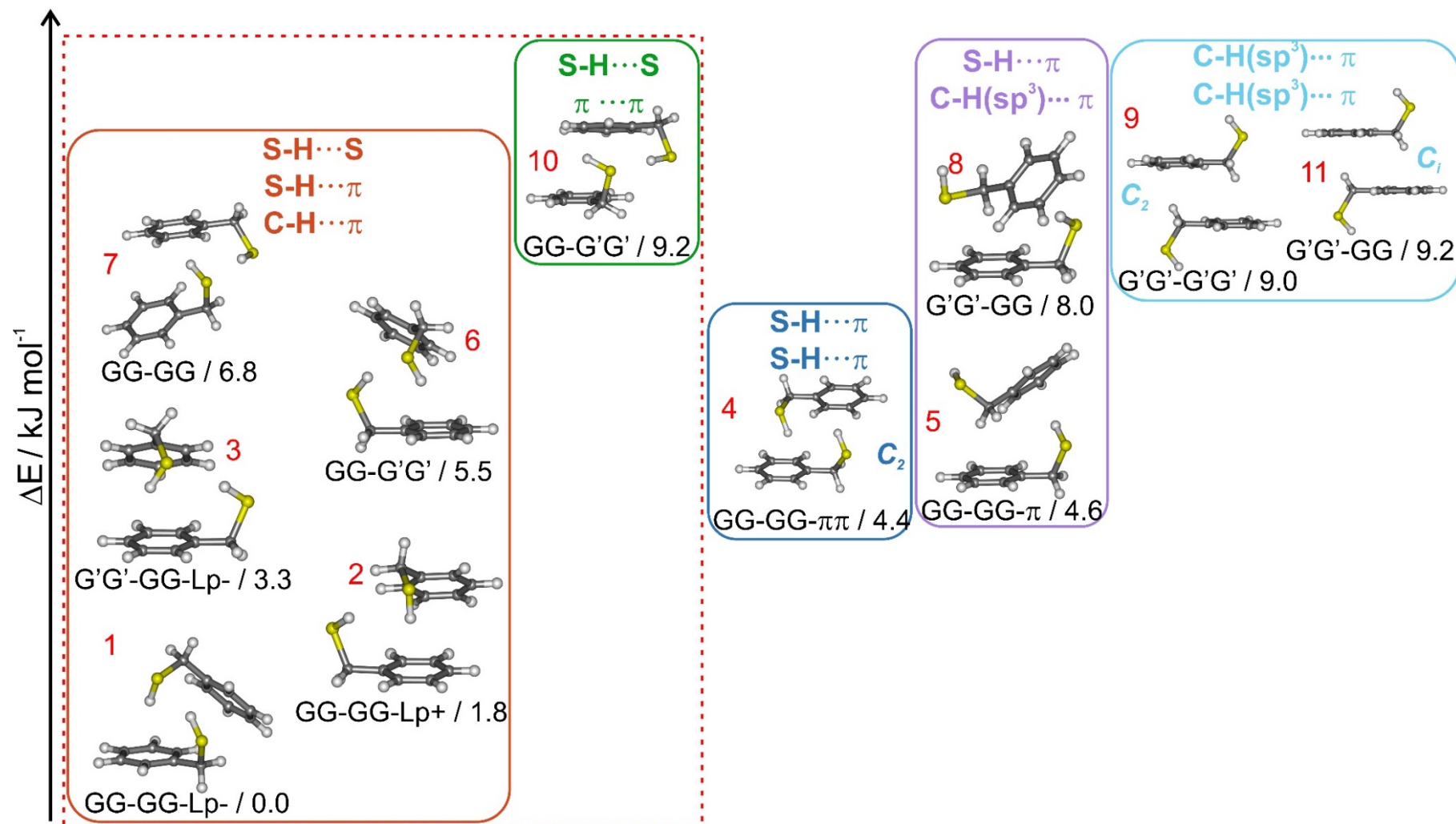
Figure S3. A rotatable 3D figure of the two most stable isomers of the benzyl mercaptan dimer.

Figure S4. A comparison of the two asymmetric (C_1) most stable isomers of the benzyl mercaptan dimer. Isomers 1 (G′G′-G′G′-Lp+ = GG-GG-Lp-, left) and 2 (G′G′-G′G′-Lp- = GG-GG-Lp+, right), are both homochiral but differ in the acceptor lone pair position of sulfur (the dihedral formed by the lone pair or τ(LpS-CαCipso) have different signs for isomer 1 and isomer 2), producing a change of relative orientation between the rings.
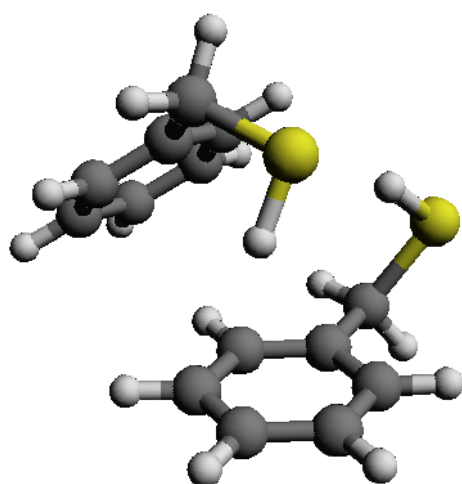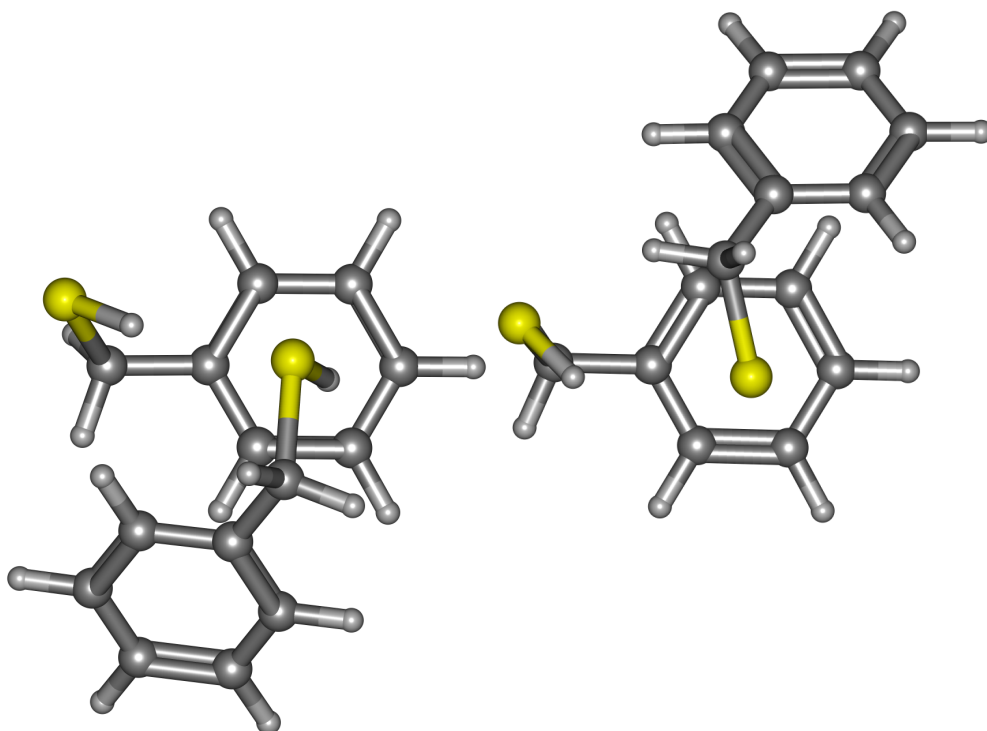
Figure S5. A comparison of the two asymmetric (C_1) most stable isomers of the benzyl mercaptan dimer. Isomers 1 (G′G′-G′G′-Lp+ = GG-GG-Lp-, left) and 3 (GG-G′G′-Lp+ = G′G′-GG-Lp-, right) differ in the stereochemistry of the donor group, either homochiral in isomer 1 or heterochiral in isomer 3.
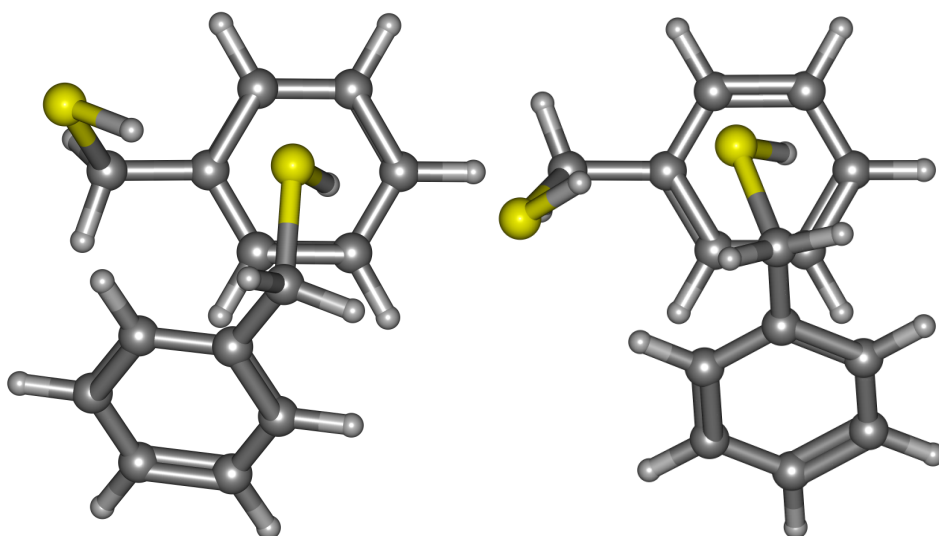
Figure S6. The most stable symmetric dimer of benzyl mercaptan (isomer 5 GG-GG-ππ) has C_2 symmetry but avoids the parallel arrangement of the two phenyl rings, unlike in the symmetric benzyl alcohol dimer. The Figure shows the (a, b, c) principal inertial axes, with a vector pointing in the C_2 ($\equiv b$) symmetry axis direction.

Figure S7. A comparison of the NCI Plots for isomers 1 (G′G′-G′G′-Lp+ = GG-GG-Lp-, upper panel) and 2 (G′G′-G′G′-Lp- = GG-GG-Lp+, lower panel) of the benzyl mercaptan dimer.
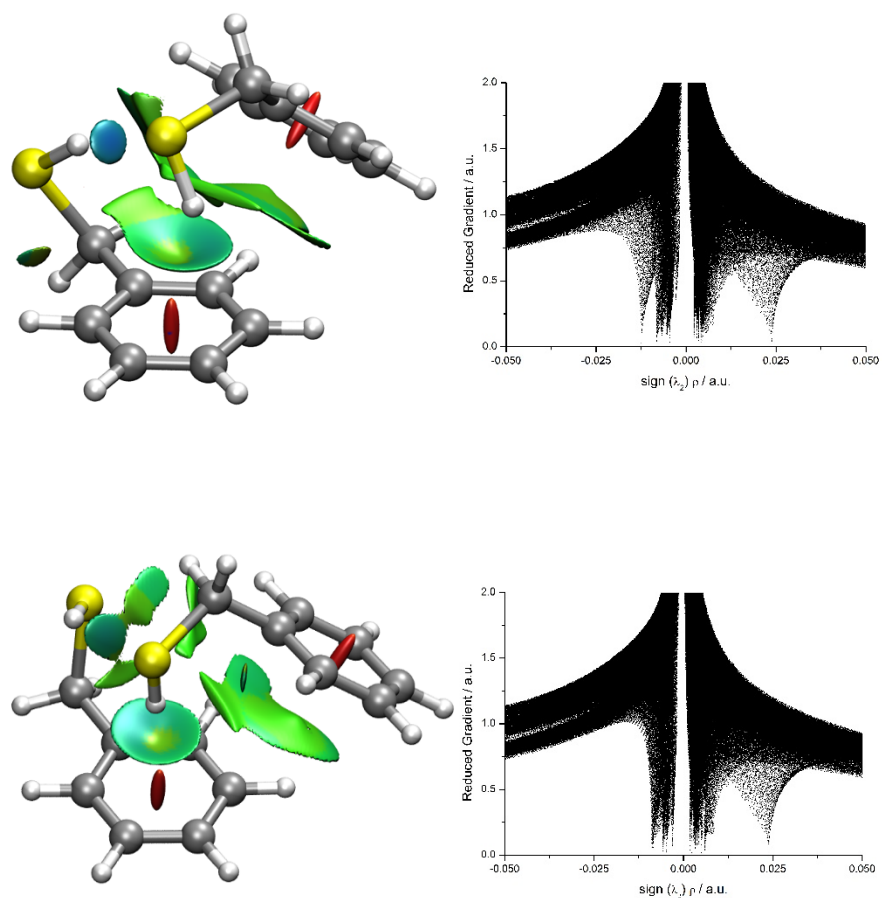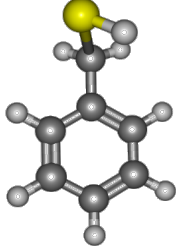
Table S1. Rotational parameters of benzyl mercaptan.

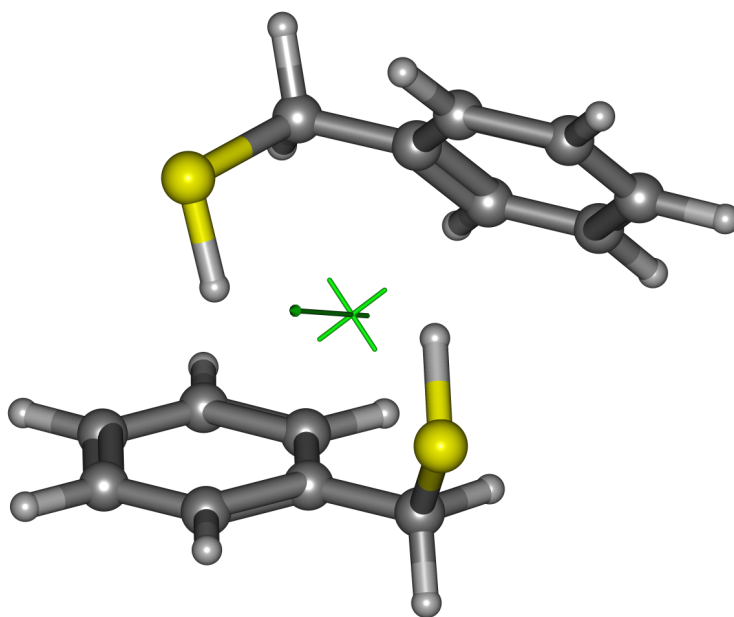|	Conformer GG		
	Experiment [a]		Theory [b]
	v=0	v=1	
A / MHz [c]	4167.4584(15) [g]	4167.7017(15)	4185.0
B / MHz	1001.61056(41)	1001.59720(36)	1000.6
C / MHz	891.69084(39)	891.65660(37)	891.0
D_J / kHz	0.1550(41)		0.127
D_{JK} / kHz [d]	2.506(22)		1.809
D_K / kHz	0.288(77)		1.726
d_1 / kHz	[0.0] [h]		0.0038
d_2 / kHz	[0.0]		0.0048
ΔE_{01} / MHz [e]	2180.4879(35)		
F_{ab} / MHz	96.3332(14)		
F_{bc} / kHz	17.88461(23)		
σ / kHz	11.5		
N	102		
μ_a / D			1.2
μ_b / D			0.6
μ_c / D			0.4
μ_{TOTAL} / D			2.0
ΔE_{ZPE} / kJ mol^{-1} [f]			0.0
ΔG / kJ mol^{-1}			0.0
HS−CαCipso / deg			53.7
SCα−CipsoCortho / deg			75.3

[a]Taken from *J. Phys. Chem. A*, **2019**, *123*, 8435–8440. [b]B3LYP-D3(BJ)/def2-TZVP. [c]Rotational constants for the first two torsional sub-states (A, B, C). [d]Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2). [e]Energy difference between the first torsional substates (ΔE_{01}), Coriolis coupling parameters (F_{ab}, F_{bc}), standard error of the fit (σ) and number of measured transitions (N). [f]Electronic energies, Gibbs energy (298 K, 1 atm) and structural parameters. [g]Standard errors in parentheses in units of the last digit. [h]Fixed to zero.

Table S2. Atomic coordinates of benzyl mercaptan *gauche* GG.

Atom [a]	a / Å	b / Å	c / Å
C	-0.0169	-0.1437	-0.4479
C	-0.7969	-1.2538	-0.1316
C	-2.1177	-1.1014	0.2762
C	-2.6742	0.1672	0.3697
C	-1.9029	1.2821	0.0542
C	-0.5849	1.1268	-0.3484
H	-0.3675	-2.2459	-0.2079
H	-2.7108	-1.9742	0.5172
H	-3.7024	0.2888	0.6846
H	-2.3313	2.2739	0.1230
H	0.0172	1.9973	-0.5785
C	1.4117	-0.3190	-0.8670
H	1.6641	0.3428	-1.6958
H	1.6015	-1.3418	-1.1873
S	2.6251	0.1323	0.4408
H	2.1100	-0.6585	1.3965

[a]Atomic coordinates in the principal axes system (a, b, c) according to B3LYP-D3(BJ)/def2-TZVP.
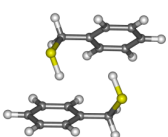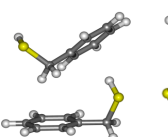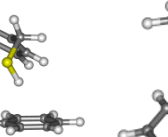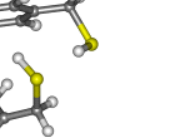
Table S3. Conformational search for the benzyl mercaptan dimer (B3LYP-D3(BJ)/def2-TZVP) and comparison with the experimental rotational parameters.

	Experiment	1	2	3
Isomer		GG-GG-Lp-	GG-GG-Lp+	G′G′-GG-Lp-
A / MHz [a]	490.79216(17) [e]	498.41	535.19	510.98
B / MHz	344.12732(12)	352.92	332.27	340.02
C / MHz	317.21115(11)	325.95	302.16	320.98
D_J / kHz	0.03861(51)	0.0323	0.0667	0.0471
D_{JK} / kHz	0.0642(18)	0.0584	-0.1183	-0.0064
D_K / kHz	-0.0718(20)	-0.0662	0.2012	0.0411
d_1 / kHz	-0.00375(33)	-0.0026	-0.0002	-0.0028
d_2 / kHz	0.00089(13)	0.0007	-0.0007	0.0007
$|\mu_a|$ / D	++	1.5	0.4	1.1
$|\mu_b|$ / D	++	1.7	1.3	1.6
$|\mu_c|$ / D	++	1.3	0.8	0.5
HBond donor [b]				
HS−CαCipso / deg		-39.62	-49.89	40.21
SCα−CipsoCortho / deg		-57.39	-70.22	64.92
HBond acceptor				
HS−CαCipso / deg		-53.09	-45.03	-44.53
SCα−CipsoCortho / deg		-67.56	-56.82	-70.87
r(S···H) / Å		2.684	2.879	2.728
∠(S−H···S) / deg		164.81	138.54	160.91
r(S−H···centroid) / Å		2.527	2.408	2.558
ΔE/ kJ mol^{-1} [c]		0.0	1.8	3.3
ΔG / kJ mol^{-1}		0.7	0.0	1.8
E_c / kJ mol^{-1}		-41.3	-38.2	-36.7
ΔE_c / kJ mol^{-1}		0.0	3.1	4.6
N [d]	337			
σ / kHz	8.5			
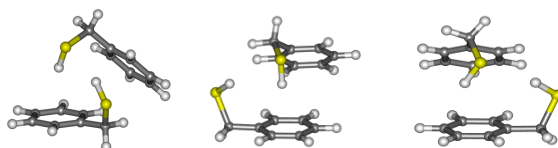
[a]Rotational constants (A, B, C), Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2) and electric dipole moments (μ_α, α = a, b, c). [b]Structural parameters of the dimer. [c]Relative electronic energies (ΔE) with zero-point correction, Gibbs energy (ΔG, 298K, 1 atm), complexation energies (E_c) and relative complexation energies (ΔE_c). [d]Number of transitions (N) and rms deviation (σ) of the fit. [e]Standard errors in units of the last digit.

Table S3. Continued.

	4	5	6	7
Isomer	GG-GG- ππ	GG-GG-π	GG-G'G'	G'G'-G'G'
A / MHz [a]	578.49	500.52	510.75	540.01
B / MHz	336.90	377.60	342.43	313.16
C / MHz	279.49	260.22	321.26	239.80
D_J / kHz	0.0444	0.0926	0.0873	0.0648
D_{JK} / kHz	-0.1414	-0.1114	0.3314	-0.1205
D_K / kHz	0.4325	0.0303	-0.0658	0.2118
d_1 / kHz	-0.0061	0.0261	-0.0075	-0.0120
d_2 / kHz	-0.0018	0.0075	0.0041	-0.0021
$|\mu_a|$ / D	0.0	0.1	0.7	0.3
$|\mu_b|$ / D	0.0	0.1	0.0	1.9
$|\mu_c|$ / D	2.2	0.4	1.6	0.2
HBond donor [b]				
HS–CαCipso / deg	-61.44	60.60	-57.58	-49.39
SCα–CipsoCortho / deg	-58.80	51.35	-60.79	-84.71
HBond acceptor				
HS–CαCipso / deg	-61.44	60.37	63.43	-64.14
SCα–CipsoCortho / deg	-58.80	73.21	87.41	-81.45
r(S···H) / Å			2.797	2.658
∠(S–H···S) / deg			162.56	154.84
r(S–H···centroid) / Å	2.521	2.482		
	2.520	2.469		
ΔE/ kJ mol^{-1} [c]	4.4	4.6	5.5	6.8
ΔG / kJ mol^{-1}	1.0	1.5	0.1	2.4
E_c / kJ mol^{-1}	-34.81	-35.65	-33.39	-32.55
ΔE_c / kJ mol^{-1}	6.44	5.61	7.87	8.70

[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]Structural parameters of the dimer. [c]Relative electronic energies (ΔE) with zero-point correction, Gibbs energy (ΔG, 298K, 1 atm), complexation energies (E_c) and relative complexation energies (ΔE_c).

Table S3. Continued.

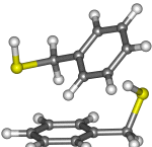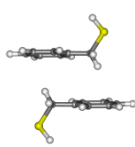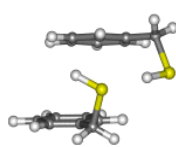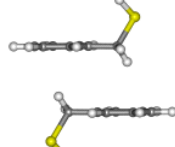|	8	9	10	11
Isomer	G′G′-GG	GG-GG	GG-G′G′	GG-G'G'
A / MHz[a]	474.03	462.48	466.32	465.46
B / MHz	346.66	361.47	400.86	357.27
C / MHz	258.85	238.73	270.71	237.28
D_J / kHz	0.1701	0.0584	0.0858	0.0461
D_{JK} / kHz	-0.2747	-0.0798	-0.1231	-0.0540
D_K / kHz	0.1359	0.0324	0.0701	0.0181
d_1 / kHz	-0.0347	-0.0072	0.0159	-0.0014
d_2 / kHz	0.0258	0.0005	0.0184	0.0043
$|\mu_a|$ / D	1.0	0.0	0.8	0.0
$|\mu_b|$ / D	0.7	0.0	1.9	0.0
$|\mu_c|$ / D	1.8	1.3	0.7	0.0
HBond donor				
HS−CαCipso / deg	-59.37	55.18	46.51	-55.26
SCα−CipsoCortho / deg	-71.38	65.43	84.25	-64.59
HBond acceptor				
HS−CαCipso / deg	56.10	55.19	-64.68	55.25
SCα−CipsoCortho / deg	71.56	65.71	-93.96	64.73
r(S···H) / Å			2.690	
∠(S–H···S) / deg			176.46	
r(S–H···centroid) / Å	2.559	2.554		
	2.647	2.552		
ΔE/ kJ mol^{-1}[c]	8.0	9.0	9.2	9.2
ΔG / kJ mol^{-1}	0.0	3.5	5.3	3.0
E_c / kJ mol^{-1}	-30.46	-30.46	-30.29	-30.08
ΔE_c / kJ mol^{-1}	10.79	10.79	10.96	11.17

[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]Structural parameters of the dimer. [c]Relative electronic energies (ΔE) with zero-point correction, Gibbs energy (ΔG, 298K, 1 atm), complexation energies (E_c) and relative complexation energies (ΔE_c).

Table S4. List of observed rotational transitions of the benzyl mercaptan dimer GG-GG-Lp- and (observed – calculated, o-c) residuals for the fit of Table 1 (all units in MHz).

	J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Freq. / MHz	o-c / MHz
1	5	1	4	4	2	3	3003.2615	0.0014
2	15	10	5	15	9	6	3014.5209	0.0033
3	15	10	6	15	9	6	3014.5209	0.0033
4	15	10	6	15	9	7	3014.5209	0.0023
5	15	10	5	15	9	7	3014.5209	0.0023
6	14	10	4	14	9	5	3019.1913	-0.0132
7	14	10	5	14	9	5	3019.1913	-0.0132
8	14	10	4	14	9	6	3019.1913	-0.0135
9	14	10	5	14	9	6	3019.1913	-0.0135
10	13	10	3	13	9	4	3023.0051	0.0021
11	13	10	4	13	9	4	3023.0051	0.0021
12	13	10	3	13	9	5	3023.0051	0.0020
13	13	10	4	13	9	5	3023.0051	0.0020
14	12	10	2	12	9	3	3026.0395	0.0009
15	12	10	2	12	9	4	3026.0395	0.0009
16	12	10	3	12	9	3	3026.0395	0.0009
17	12	10	3	12	9	4	3026.0395	0.0009
18	11	10	1	11	9	2	3028.4302	0.0055
19	11	10	1	11	9	3	3028.4302	0.0055
20	11	10	2	11	9	2	3028.4302	0.0055
21	11	10	2	11	9	3	3028.4302	0.0055
22	4	2	3	3	1	2	3044.5916	0.0067
23	4	2	2	3	1	2	3092.0905	0.0037
24	5	0	5	4	1	4	3185.8517	-0.0026
25	4	2	3	3	1	3	3205.8200	0.0063
26	5	1	5	4	1	4	3227.1334	0.0039
27	5	0	5	4	0	4	3250.8942	-0.0060
28	4	2	2	3	1	3	3253.3122	-0.0034
29	5	1	5	4	0	4	3292.1765	0.0011
30	5	2	4	4	2	3	3299.1824	0.0032
31	5	3	3	4	3	2	3315.7372	0.0020
32	5	3	2	4	3	1	3321.1660	0.0044
33	5	2	3	4	2	2	3354.8164	0.0026
34	5	1	4	4	1	3	3356.2760	-0.0030
35	4	3	2	3	2	1	3437.4243	-0.0059
36	4	3	1	3	2	1	3439.2828	-0.0005
37	6	0	6	5	1	4	3445.8361	0.0015
38	4	3	2	3	2	2	3453.9662	-0.0039
39	4	3	1	3	2	2	3455.8224	-0.0008
40	6	1	5	5	2	3	3615.2616	-0.0016
41	5	2	4	4	1	3	3652.1950	-0.0031
42	6	1	5	5	2	4	3718.4073	0.0076
43	7	2	6	6	3	3	3727.7143	0.0075
44	7	2	6	6	3	4	3748.8557	0.0072
45	5	2	3	4	1	3	3755.3324	-0.0022
46	4	4	1	3	3	0	3766.6115	0.0317
47	4	4	0	3	3	0	3766.6115	0.0142
48	4	4	1	3	3	1	3766.8209	-0.0259
49	4	4	0	3	3	1	3766.8209	-0.0434
50	6	0	6	5	1	5	3842.2952	0.0053
51	6	0	6	5	0	5	3883.5613	-0.0036
52	6	1	6	5	0	5	3907.9721	-0.0036
53	5	2	4	4	1	4	3919.5039	0.0001

54	7	0	7	6	1	5	3946.7814	0.0076
55	6	2	5	5	2	4	3952.9727	0.0031
56	6	5	2	5	5	1	3976.4830	0.0084
57	6	5	1	5	5	0	3976.4830	-0.0018
58	6	4	3	5	4	2	3979.2657	-0.0042
59	6	4	2	5	4	1	3979.8814	-0.0069
60	6	3	4	5	3	3	3980.0476	0.0026
61	6	1	5	5	1	4	4014.3151	-0.0037
62	5	2	3	4	1	4	4022.6428	0.0025
63	7	2	5	6	3	3	4026.6949	-0.0046
64	6	2	4	5	2	3	4036.7867	0.0015
65	7	2	5	6	3	4	4047.8348	-0.0064
66	5	3	3	4	2	2	4079.4920	-0.0052
67	5	3	2	4	2	2	4086.7772	0.0003
68	5	3	3	4	2	3	4126.9947	-0.0045
69	5	3	2	4	2	3	4134.2751	-0.0036
70	8	3	6	7	4	3	4187.6106	0.0057
71	8	3	6	7	4	4	4190.4011	0.0018
72	7	1	6	6	2	4	4242.4017	-0.0094
73	6	2	5	5	1	4	4248.8924	0.0037
74	8	3	5	7	4	3	4289.2450	-0.0026
75	8	3	5	7	4	4	4292.0301	-0.0118
76	8	2	7	7	3	4	4306.5833	0.0101
77	8	2	7	7	3	5	4356.6804	0.0048
78	5	4	2	4	3	1	4427.7774	-0.0076
79	5	4	1	4	3	1	4427.9448	0.0031
80	7	1	6	6	2	5	4429.3670	0.0038
81	5	4	2	4	3	2	4429.6300	-0.0080
82	5	4	1	4	3	2	4429.7914	-0.0033
83	8	0	8	7	1	6	4430.2471	0.0101
84	6	2	4	5	1	4	4435.8365	-0.0041
85	6	1	5	5	0	5	4452.0459	-0.0031
86	7	0	7	6	1	6	4490.8489	0.0018
87	7	1	7	6	1	6	4504.5425	-0.0045
88	7	0	7	6	0	6	4515.2606	0.0026
89	7	1	7	6	0	6	4528.9541	-0.0038
90	7	2	6	6	2	5	4603.7446	0.0007
91	7	6	2	6	6	1	4638.8036	0.0000
92	7	6	1	6	6	0	4638.8036	-0.0006
93	7	5	3	6	5	2	4641.3749	0.0295
94	7	5	2	6	5	1	4641.3749	-0.0266
95	7	3	5	6	3	4	4643.5319	0.0044
96	6	2	5	5	1	5	4645.3486	0.0046
97	7	4	4	6	4	3	4645.3486	-0.0016
98	7	4	3	6	4	2	4647.3668	-0.0027
99	7	1	6	6	1	5	4663.9357	0.0026
100	7	3	4	6	3	3	4672.4861	-0.0019
101	6	3	4	5	2	3	4704.7221	-0.0064
102	7	2	5	6	2	4	4715.7847	0.0000
103	6	3	3	5	2	3	4725.8724	0.0021
104	8	2	6	7	3	4	4743.4250	0.0027
105	5	5	0	4	4	0	4748.3134	0.0006
106	5	5	1	4	4	1	4748.3134	-0.0158
107	5	5	0	4	4	1	4748.3134	-0.0168
108	5	5	1	4	4	0	4748.3134	0.0016
109	8	2	6	7	3	5	4793.5157	-0.0089
110	6	3	4	5	2	4	4807.8591	-0.0058
111	6	3	3	5	2	4	4829.0107	0.0040
112	8	1	7	7	2	5	4831.2734	-0.0018
113	6	2	4	5	1	5	4832.3096	0.0137

114	9	3	7	8	4	4	4834.7929	0.0177
115	7	2	6	6	1	5	4838.3163	0.0025
116	9	2	8	8	3	5	4845.5509	-0.0103
117	9	2	8	8	3	6	4947.1922	-0.0117
118	9	3	6	8	4	4	5016.4674	-0.0199
119	9	3	6	8	4	5	5024.6695	0.0125
120	6	4	3	5	3	2	5085.8942	0.0007
121	6	4	2	5	3	2	5086.6639	-0.0045
122	6	4	3	5	3	3	5093.1698	-0.0032
123	6	4	2	5	3	3	5093.9489	0.0009
124	8	1	7	7	2	6	5130.2654	-0.0026
125	8	0	8	7	1	7	5133.6896	-0.0066
126	7	2	5	6	1	5	5137.3045	-0.0020
127	8	1	8	7	1	7	5141.0997	0.0024
128	8	0	8	7	0	7	5147.3971	0.0008
129	8	1	8	7	0	7	5154.7984	0.0011
130	7	1	6	6	0	6	5232.4199	0.0026
131	8	2	7	7	2	6	5251.3574	0.0028
132	10	4	6	9	5	4	5273.3971	-0.0101
133	10	4	6	9	5	5	5274.3958	-0.0091
134	8	7	2	7	7	1	5301.1412	-0.0136
135	8	7	1	7	7	0	5301.1412	-0.0136
136	8	6	3	7	6	2	5303.4211	0.0017
137	8	6	2	7	6	1	5303.4211	-0.0026
138	10	1	10	9	2	8	5304.6487	0.0169
139	8	1	7	7	1	6	5304.6487	0.0000
140	8	3	6	7	3	5	5305.3427	-0.0072
141	8	5	4	7	5	3	5307.1644	-0.0050
142	8	5	3	7	5	2	5307.3872	-0.0043
143	7	3	5	6	2	4	5311.4709	0.0000
144	8	4	5	7	4	4	5312.1987	0.0016
145	8	4	4	7	4	3	5317.5739	0.0015
146	10	2	9	9	3	6	5338.3431	-0.0190
147	8	3	5	7	3	4	5356.8888	-0.0015
148	7	3	4	6	2	4	5361.5681	-0.0050
149	9	1	8	8	2	6	5380.2760	0.0083
150	7	2	6	6	1	6	5382.3903	0.0033
151	8	2	6	7	2	5	5389.2127	0.0018
152	6	5	2	5	4	1	5410.6007	0.1072
153	6	5	1	5	4	1	5410.6007	0.0959
154	6	5	2	5	4	2	5410.6007	-0.0493
155	6	5	1	5	4	2	5410.6007	-0.0607
156	8	2	7	7	1	6	5425.7348	-0.0003
157	9	2	7	8	3	5	5441.7897	0.0041
158	10	3	8	9	4	5	5464.2155	0.0053
159	10	3	8	9	4	6	5484.6500	-0.0014
160	7	3	5	6	2	5	5498.4157	-0.0071
161	9	2	7	8	3	6	5543.4257	-0.0026
162	7	3	4	6	2	5	5548.5234	-0.0017
163	7	2	5	6	1	6	5681.3750	-0.0047
164	6	6	0	5	5	0	5729.9000	-0.0007
165	6	6	1	5	5	0	5729.9000	-0.0006
166	6	6	1	5	5	1	5729.9000	-0.0016
167	6	6	0	5	5	1	5729.9000	-0.0017
168	7	4	4	6	3	3	5737.3353	-0.0011
169	7	4	3	6	3	3	5740.1292	-0.0016
170	7	4	4	6	3	4	5758.4762	-0.0020
171	7	4	3	6	3	4	5761.2709	-0.0016
172	9	0	9	8	1	8	5772.8719	0.0015
173	9	1	9	8	1	8	5776.7579	0.0006

174	9	0	9	8	0	8	5780.2723	0.0008
175	9	1	9	8	0	8	5784.1599	0.0016
176	9	1	8	8	2	7	5817.1198	0.0030
177	8	2	6	7	1	6	5862.5846	0.0002
178	9	2	8	8	2	7	5895.8790	0.0004
179	8	3	6	7	2	5	5901.0342	-0.0020
180	9	1	8	8	1	7	5938.2024	-0.0008
181	9	8	1	8	8	0	5963.5282	0.0135
182	9	8	2	8	8	1	5963.5282	0.0135
183	9	3	7	8	3	6	5964.7421	-0.0005
184	9	7	3	8	7	2	5965.5889	0.0026
185	9	7	2	8	7	1	5965.5889	0.0022
186	9	6	4	8	6	3	5968.8228	0.0095
187	9	6	3	8	6	2	5968.8228	-0.0110
188	9	5	5	8	5	4	5974.0271	0.0047
189	9	5	4	8	5	3	5974.7323	0.0020
190	9	4	6	8	4	5	5979.3893	0.0022
191	9	4	5	8	4	4	5991.6619	0.0032
192	8	3	5	7	2	5	6002.6789	0.0000
193	9	2	8	8	1	7	6016.9657	0.0007
194	8	1	7	7	0	7	6021.8079	-0.0001
195	9	3	6	8	3	5	6044.8152	0.0031
196	9	2	7	8	2	6	6055.2540	0.0003
197	11	3	9	10	4	6	6067.2722	-0.0010
198	7	5	3	6	4	2	6071.9911	0.0406
199	7	5	2	6	4	2	6071.9911	-0.0269
200	7	5	3	6	4	3	6072.7545	0.0291
201	7	5	2	6	4	3	6072.7545	-0.0384
202	10	2	8	9	3	6	6109.3442	0.0053
203	11	3	9	10	4	7	6112.3660	-0.0180
204	8	2	7	7	1	7	6129.1956	0.0011
205	8	3	6	7	2	6	6200.0285	-0.0005
206	10	2	8	9	3	7	6291.0537	0.0027
207	8	3	5	7	2	6	6301.6712	-0.0005
208	8	4	5	7	3	4	6377.0441	-0.0014
209	11	1	10	10	2	8	6377.5971	0.0091
210	8	4	4	7	3	4	6385.2135	-0.0016
211	7	6	2	6	5	1	6392.2237	0.0044
212	7	6	1	6	5	1	6392.2237	0.0037
213	7	6	2	6	5	2	6392.2237	-0.0068
214	7	6	1	6	5	2	6392.2237	-0.0076
215	10	0	10	9	1	9	6409.8507	-0.0017
216	10	1	10	9	1	9	6411.8499	-0.0003
217	10	0	10	9	0	9	6413.7382	-0.0012
218	10	1	10	9	0	9	6415.7383	0.0012
219	8	4	5	7	3	5	6427.1475	-0.0003
220	8	4	4	7	3	5	6435.3135	-0.0039
221	9	3	7	8	2	6	6476.5693	0.0012
222	10	1	9	9	2	8	6489.1920	0.0009
223	10	2	9	9	2	8	6537.6126	-0.0003
224	10	1	9	9	1	8	6567.9525	-0.0003
225	9	2	7	8	1	7	6613.1891	-0.0001
226	10	2	9	9	1	8	6616.3744	-0.0003
227	10	3	8	9	3	7	6621.0959	0.0022
228	10	9	1	9	9	0	6625.8754	0.0021
229	10	9	2	9	9	1	6625.8754	0.0021
230	10	8	2	9	8	1	6627.8139	0.0036
231	10	8	3	9	8	2	6627.8139	0.0036
232	10	7	4	9	7	3	6630.6600	0.0048
233	10	7	3	9	7	2	6630.6600	0.0031

234	10	6	5	9	6	4	6635.0964	0.0127
235	10	6	4	9	6	3	6635.0964	-0.0632
236	10	5	6	9	5	5	6641.9018	0.0001
237	10	5	5	9	5	4	6643.8320	0.0021
238	10	4	7	9	4	6	6646.2774	0.0002
239	9	3	6	8	2	6	6658.2804	0.0002
240	10	4	6	9	4	5	6670.9478	0.0010
241	7	7	0	6	6	0	6711.4711	-0.0004
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245	10	2	8	9	2	7	6712.3680	0.0026
246	12	3	10	11	4	8	6723.6521	-0.0105
247	8	5	4	7	4	3	6731.7504	0.0000
248	8	5	3	7	4	3	6732.0418	0.0017
249	10	3	7	9	3	6	6732.1948	0.0020
250	8	5	4	7	4	4	6734.5440	-0.0007
251	8	5	3	7	4	4	6734.8363	0.0019
252	11	2	9	10	3	7	6736.6271	-0.0073
253	9	1	8	8	0	8	6812.6083	-0.0066
254	9	2	8	8	1	8	6883.9767	0.0010
255	9	3	7	8	2	7	6913.4201	0.0029
256	9	4	6	8	3	5	6999.5390	-0.0030
257	9	4	5	8	3	5	7019.9815	-0.0018
258	11	2	9	10	3	8	7029.4558	0.0101
259	10	3	8	9	2	7	7042.4135	0.0054
260	11	0	11	10	1	10	7045.5979	0.0042
261	11	1	11	10	1	10	7046.6029	-0.0002
262	11	0	11	10	0	10	7047.5909	-0.0005
263	11	1	11	10	0	10	7048.6010	0.0002
264	8	6	3	7	5	2	7054.2223	-0.0147
265	8	6	2	7	5	2	7054.2223	-0.0199
266	8	6	3	7	5	3	7054.3306	0.0260
267	8	6	2	7	5	3	7054.3306	0.0208
268	9	3	6	8	2	7	7095.1352	0.0058
269	9	4	6	8	3	6	7101.1851	0.0002
270	9	4	5	8	3	6	7121.6265	0.0004
271	11	1	10	10	2	9	7148.5627	-0.0019
272	11	2	10	10	2	9	7177.0174	0.0000
273	11	1	10	10	1	9	7196.9882	0.0016
274	11	3	9	10	3	8	7274.0089	-0.0008
275	11	10	1	10	10	0	7288.2200	-0.0042
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277	11	9	2	10	9	1	7290.0757	0.0123
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279	11	8	4	10	8	3	7292.6484	0.0064
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281	11	7	5	10	7	4	7296.4523	0.0139
282	11	7	4	10	7	3	7296.4523	0.0068
283	11	6	5	10	6	4	7302.5626	0.0040
284	11	5	7	10	5	6	7310.6874	0.0084
285	11	4	8	10	4	7	7312.0753	0.0058
286	11	5	6	10	5	5	7315.3237	0.0058
287	13	3	11	12	4	9	7316.9676	0.0015
288	12	2	10	11	3	8	7318.5871	0.0059
289	10	3	7	9	2	7	7335.2196	0.0004
290	11	4	7	10	4	6	7356.3000	0.0046
291	11	2	9	10	2	8	7359.4913	0.0030
292	8	7	1	7	6	1	7373.8236	0.0012
293	8	7	2	7	6	1	7373.8236	0.0012

294	8	7	2	7	6	2	7373.8236	0.0005
295	8	7	1	7	6	2	7373.8236	0.0004
296	10	2	8	9	1	8	7387.3579	0.0064
297	9	5	5	8	4	4	7388.2018	0.0014
298	9	5	4	8	4	4	7389.1990	0.0009
299	9	5	5	8	4	5	7396.3694	-0.0006
300	9	5	4	8	4	5	7397.3677	0.0000
301	11	3	8	10	3	7	7415.0239	0.0057
302	10	1	9	9	0	9	7600.3019	0.0056
303	10	4	7	9	3	6	7601.0025	-0.0047
304	11	3	9	10	2	8	7604.0504	-0.0019
305	10	3	8	9	2	8	7638.6375	0.0052
306	10	2	9	9	1	9	7644.8406	0.0092
307	10	4	6	9	3	6	7646.1130	-0.0050
308	12	0	12	11	1	11	7680.6587	0.0006
309	12	1	12	11	1	11	7681.1604	-0.0005
310	12	0	12	11	0	11	7681.6648	-0.0025
311	12	1	12	11	0	11	7682.1710	0.0006
312	8	8	0	7	7	0	7693.0346	0.0003
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316	9	6	4	8	5	3	7715.7114	0.0526
317	9	6	3	8	5	3	7715.7114	0.0269
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320	12	2	10	11	3	9	7752.3950	-0.0057
321	10	4	7	9	3	7	7782.7155	-0.0038
322	12	1	11	11	2	10	7798.4859	0.0037
323	12	2	11	11	2	10	7814.6236	0.0011
324	12	1	11	11	1	10	7826.9380	0.0031
325	10	4	6	9	3	7	7827.8263	-0.0038
326	12	2	11	11	1	10	7843.0747	-0.0004
327	12	3	10	11	3	9	7923.3558	0.0077
328	12	8	5	11	8	4	7958.0592	-0.0090
329	12	8	4	11	8	3	7958.0592	-0.0096
330	12	7	6	11	7	5	7963.0388	0.0233
331	12	7	5	11	7	4	7963.0388	-0.0018
332	12	6	7	11	6	6	7970.5159	-0.0700
333	12	6	6	11	6	5	7971.2473	0.0013
334	12	4	9	11	4	8	7975.9171	-0.0001
335	12	5	8	11	5	7	7980.0593	0.0049
336	12	5	7	11	5	6	7990.1175	0.0079
337	12	2	10	11	2	9	7996.9715	0.0066