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Supporting Information

The Role of Non-Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane

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At the end of the file, the complete set of rotational transitions for all the DFM clusters observed are provided as separated files, in the following order: 5-I, 6-I, 6-II, 7-II.

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1 Experimental Results

1.1 Experimental Details

The microwave spectra of DFM were registered in Pate's group at the University of Virginia using a CP-FTMW spectrometer, which covers the frequency ranges 2–8 GHz, while the upper spectra were measured by means of the CP-FTMW in Cocinero's group at the University of the Basque Country (UPV/EHU), which covers the frequency range 6-18 GHz. Both equipment were already described in details elsewhere.[1–3] The experiment in Virginia was carried out using 5 nozzles at the same time, and applying 8 chirps for each molecular pulse. On the other hand, the Bilbao's experiment was performed with 3 nozzles at the same time, and using 20 chirps for each molecular pulse. For the first spectrum, the number of final acquisitions is 3 million and 200 thousands, while for the second one registered in Bilbao it is 5 million.
The DFM sample was obtained from Sigma Aldrich. In both experiments, a gas mixture of ~1% CH_2F_2 in Ne was used at a backing pressure of 350 kPa, and then adiabatically expanded into the spectrometer by a few hundred μs duration pulses.

1.2 Fit results

The final fits were performed using Pickett's program, and all rotational frequencies were fitted with a Watson *S*-reduced Hamiltonian in the I^r representation.[4] The errors in parenthesis are in units of the last digit. σ is the root-mean-square deviation of the fit. *N* is the number of distinct frequency lines in the fit. The complete set of rotational transitions together with the fit results are given at the end of this Supporting Information file.

Table S1. Spectroscopic parameters obtained for the DFM clusters observed.

	5-I	**6-I**	**6-II**	**7-II**
A/MHz	426.61950(7)	356.1116(7)	304.72043(7)	229.5257(1)
B/MHz	358.42855(5)	211.52526(4)	266.17778(5)	215.0008(1)
C/MHz	281.54415(5)	185.23390(5)	226.35912(5)	163.3655(1)
D_J/kHz	0.0961(1)	0.02118(5)	0.0207(1)	0.0084(3)
D_{JK}/kHz	-0.0405(7)	0.0135(4)	0.0580(5)	0.068(1)
D_K /kHz	0.0706(6)	0.33(2)	-0.0374(5)	-0.055(1)
d_1/kHz	-0.02690(5)	[0.][a]	-0.00175(5)	-0.0028(1)
d_2/kHz	-0.00306(3)	-0.00076(3)	-0.00173(3)	-0.00318(8)
μ_a	weak	strong	medium	medium
μ_b	strong	weak	-	strong
μ_c	medium	-	weak	weak
N	474	328	385	348
σ /kHz	8.1	8.2	6.2	9.7

[a] Fixed to zero.

1.2.1 6-I Details of Assignment

The assignment of cluster 6-I is based not only on the values of the rotational constants and on its maximum energy stability, but also on the type of lines observed in the spectrum. To avoid possible assignment doubts with the 6-VI isomer (see the following figures and tables), the very few observed μ_b-lines belonging to 6-I are reported. μ_b-lines are present in the spectrum (see the following picture) since predicted more than 20 times weaker with respect to the μ_a, but their intensity touches the limit of detections, so even if their S/N is much less than 4 (the threshold chosen by the authors to measure lines), the authors decided to include them anyway. On the other hand, the μ_b-lines of the 6-VI cluster are predicted more than 300 times weaker, so for sure not detectable at all. Moreover, the μ_c-lines of 6-VI were not observed and they should be stronger that μ_b and only 38 times weaker than μ_a -lines observed of 6-I. All these considerations support the 6-I assignment.

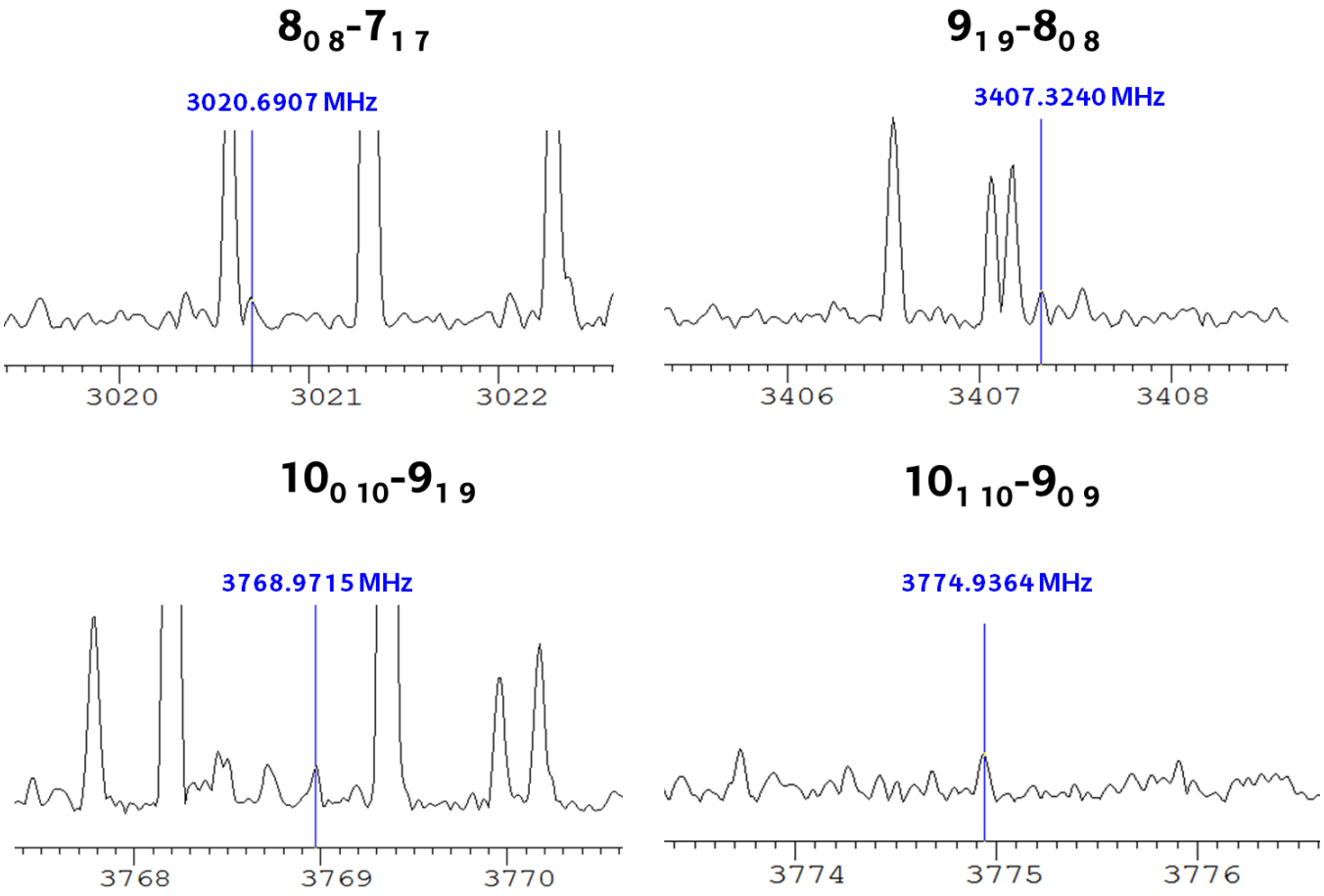
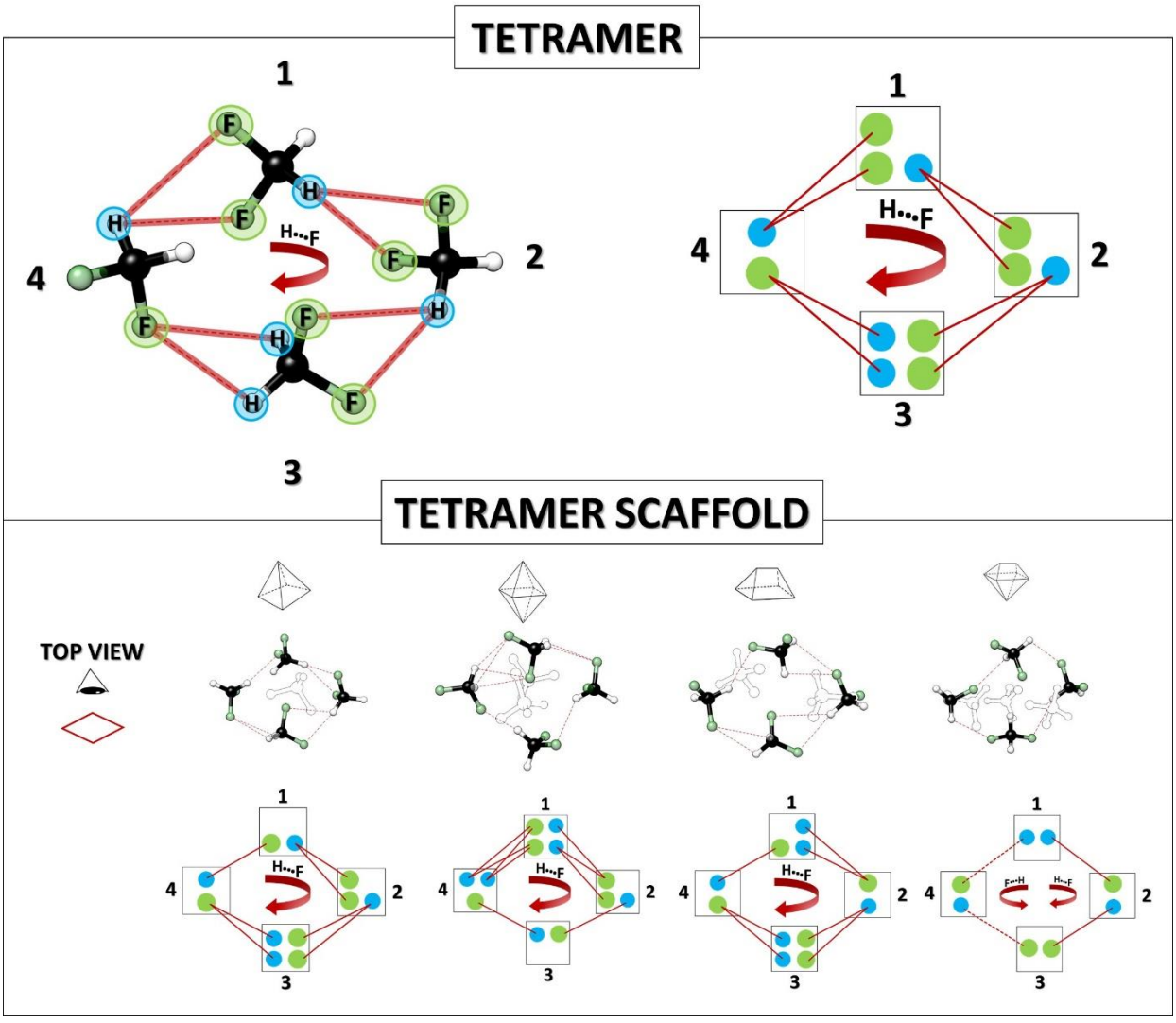


Figure S1. Observed μ_b-transitions belonging to cluster 6-I but not included in the fit due to their low S/N ratio.

1.3 Structural Analysis

For each observed structure for (DFM)n, with n ≥ 4, the analysis of the WHB was performed taking into account the 2.3 Å < CH···F ≤ 2.9 Å range. The following tables contain the complete list of intermolecular interactions for each cluster. The structures of the DFM clusters were computed at MP2/VTZ-F12 level of theory. The color code of the CH···F interactions follow the criteria described in the paper: (red lines) interactions belong to the rhomboid circular structure which resemble the tetramer one; (purple lines) other interactions inside the tetramer scaffold; (yellow lines) interactions of the upper vertices with the tetramer scaffold; (blue lines) CH···F contacts involving the lower vertices and the tetramer scaffold, and (green lines) interactions between the higher vertices that do not involve the rhomboid circular structure.

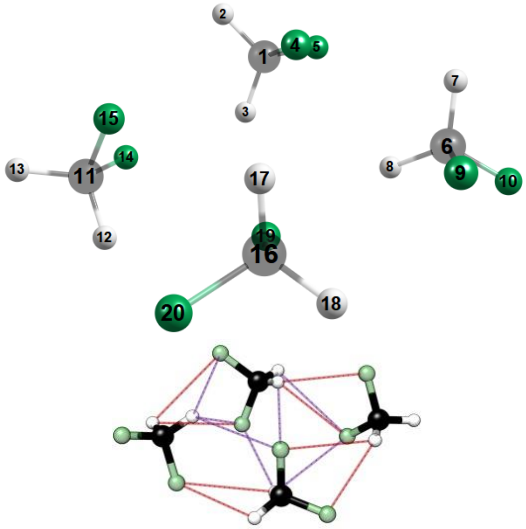
Moreover, in the following sketch, intuitive schemes of the principal CH···F interactions involved in the tetramer scaffold are shown.



Sketch 1: The interactions characterizing the tetramer (upper panel) are schematized in order to make them more identifiable in the larger clusters (lower panel).

Table S2. List of the 2.3 Å < CH···F ≤ 2.9 Å for the 4-III structure

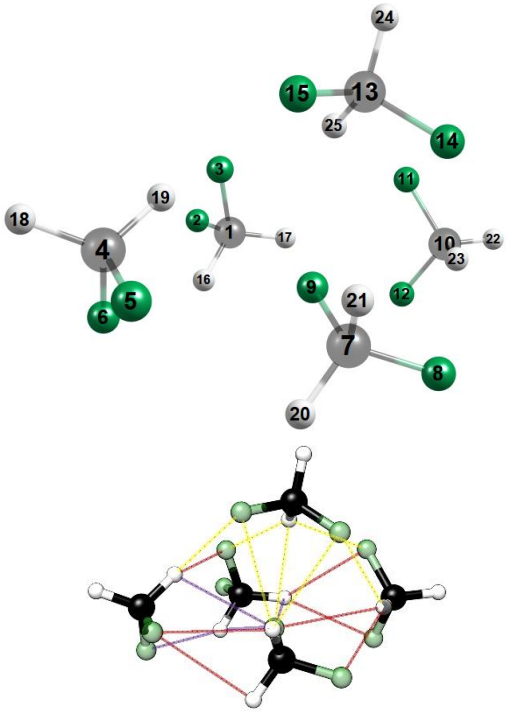
4-III



F	H	Å
20	12	2.459
19	3	2.502
4	17	2.520
14	3	2.539
9	18	2.557
19	8	2.607
19	12	2.661
15	3	2.671
15	17	2.761
4	7	2.768
4	8	2.848
9	17	2.851
5	8	2.868
5	7	2.881
15	2	2.986

Table S3. List of the 2.3 Å < CH···F ≤ 2.9 Å for the 5-I structure

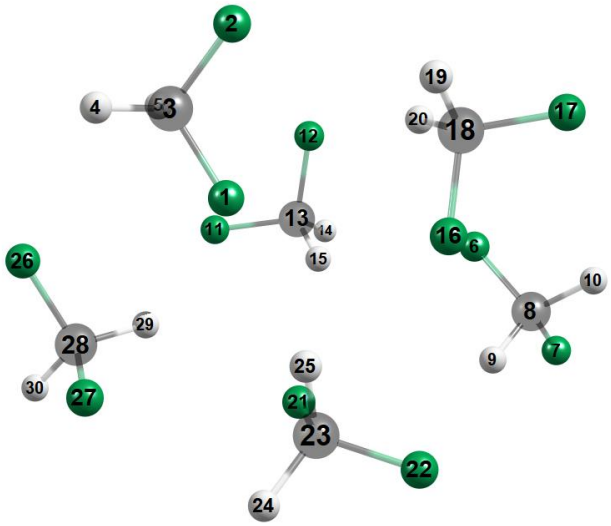
5-I

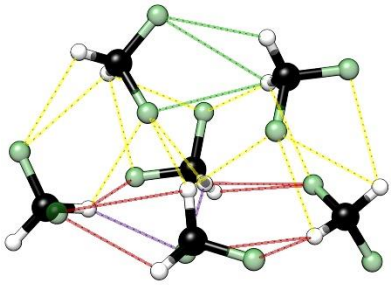


F	H	Å
3	25	2.375
8	23	2.408
3	19	2.434
11	25	2.441
6	16	2.464
15	19	2.477
12	17	2.499
14	23	2.564
9	25	2.572
11	17	2.575
9	23	2.611
9	19	2.619
14	21	2.687
9	16	2.690
5	21	2.690
5	20	2.718
15	21	2.736
9	17	2.880

Table S4. List of the 2.3 Å < CH···F ≤ 2.9 Å for the 6-I structure

6-I

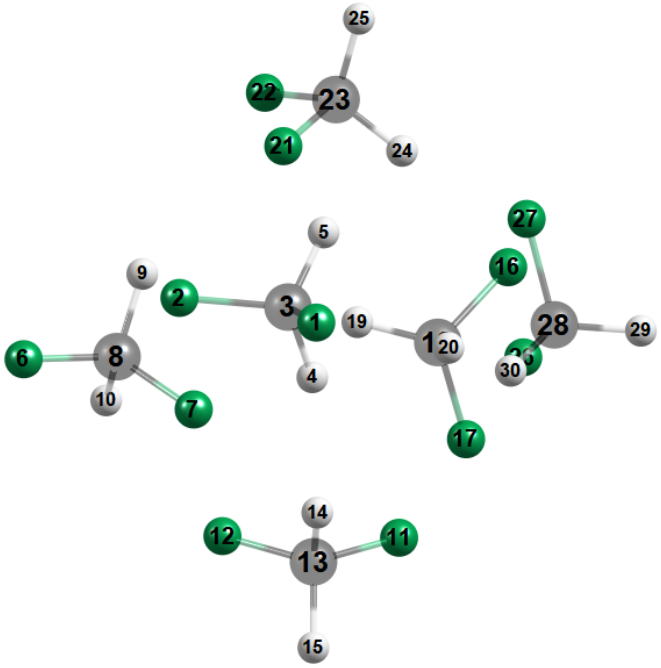


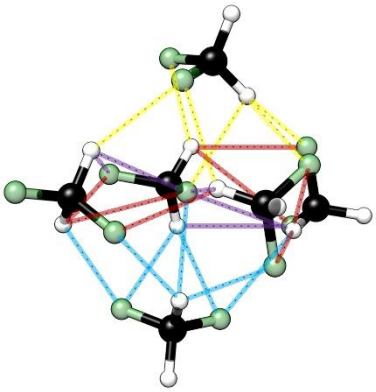


F	H	Å	F	H	Å
21	15	2.333	27	24	2.655
11	29	2.367	6	20	2.686
12	20	2.376	2	19	2.704
16	25	2.455	17	10	2.734
22	9	2.471	11	5	2.737
1	25	2.509	6	14	2.776
6	15	2.524	27	25	2.892
21	29	2.544	16	10	2.894
1	15	2.562	26	5	2.901
26	4	2.612	21	9	2.909
1	29	2.621	2	20	2.957
16	9	2.628	1	20	2.961
12	5	2.655			

Table S5. List of the 2.3 Å < CH···F ≤ 2.9 Å for the 6-II structure

6-II

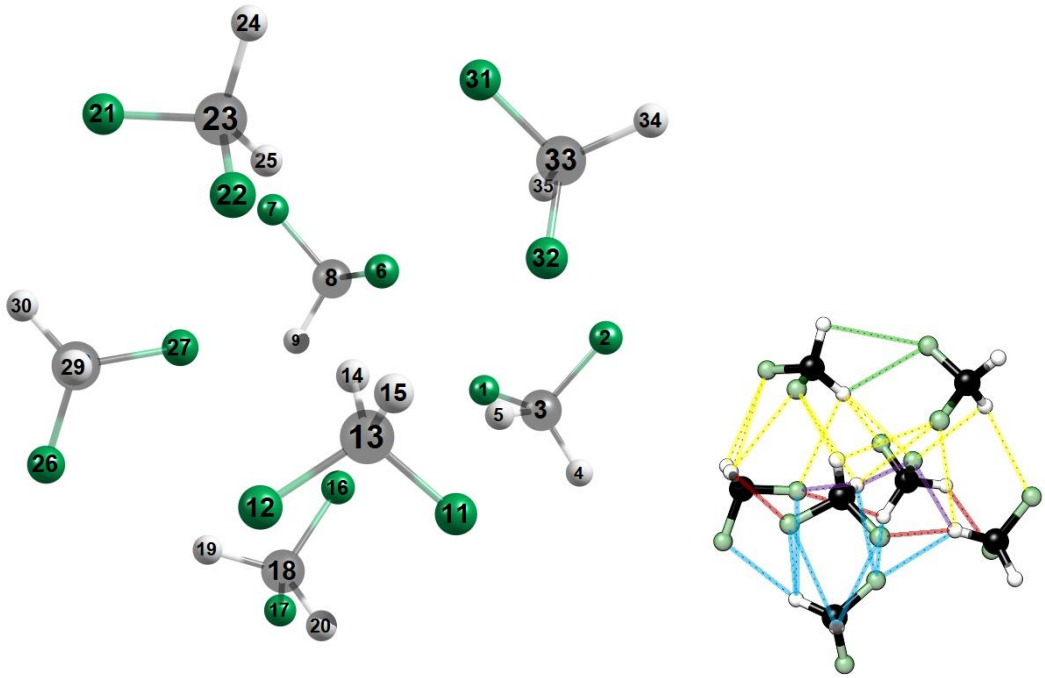




F	H	Å	F	H	Å
7	19	2.334	22	5	2.612
27	24	2.354	11	4	2.615
17	14	2.418	2	10	2.616
21	19	2.418	1	14	2.616
7	14	2.427	12	4	2.668
16	24	2.474	26	4	2.679
21	9	2.498	16	30	2.719
1	30	2.525	1	9	2.732
17	30	2.534	27	5	2.754
1	19	2.563	1	10	2.907
1	24	2.566	2	9	2.946
12	10	2.574	26	5	2.996
11	30	2.605			

Table S6. List of the 2.3 Å < CH···F ≤ 2.9 Å for the 7-II structure

7-II



F	H	Å	F	H	Å
6	14	2.379	22	29	2.655
6	25	2.402	16	14	2.655
26	19	2.411	21	30	2.661
16	9	2.427	22	15	2.661
6	35	2.464	27	25	2.667
2	35	2.472	32	15	2.672
11	5	2.488	22	14	2.696
27	14	2.498	11	20	2.731
16	5	2.506	31	24	2.731
27	9	2.515	27	19	2.758
7	25	2.559	12	20	2.760
1	10	2.565	31	25	2.766
6	5	2.568	12	19	2.809
12	29	2.592	32	5	2.824
32	14	2.640	21	29	2.953

2 Computations

2.1 Structure Determination

2.1.1 Genetic Algorithm Search on Semi-empirical PES[S4]

Determining the structure of the most stable molecular clusters is challenging because it requires an accurate potential energy surface (PES). This is particularly difficult for weakly bound clusters like those composed of DFM.

To overcome these challenges, we employed a genetic algorithm (GA)[6] approach on semi-empirical PES. The GA approach is implemented in the OGOLEM[7] package which interfaces with the PM7[8] method implemented in MOPAC[9] and the HF-3c[10] method implemented in ORCA.[11]

The details of the GA runs are summarized in Table S7.

Table S7.Details of GA runs for $(CH_2F_2)_n$, where n = 2 − 7

	GA package	SE package	Method	Pool size[a]	Number of cycles[b]
n=2-4	OGOLEM	MOPAC	PM7	50-100	2,000 - 5,000
	OGOLEM	ORCA	HF-3c	20-50	1,000
n=5-7	OGOLEM	MOPAC	PM7	500	20,000
	OGOLEM	ORCA	HF-3c	250	5,000

[a] The size of the initial and/or maintained population.

[b] Number of matings or cycles for which the population is evolved.

GA searches on semi-empirical (PM7, HF-3c) PESs yield a large number of stable isomers which are subsequently subject to refinements using more robust *ab initio* methods.

2.1.2 Refinements using *ab initio* Methods

The low energy isomers from the previous step that are within 5 kcal mol^{-1} of the putative global minimum for each method (PM7, HF-3c) are first optimized using second-order Møller-Plesset perturbation theory (MP2) with a split-valence 6-31+G(d) basis set. Those isomers that are within 3 kcal mol^{-1} of the MP2/6-31+G(d) global minimum are further optimized using the larger double-zeta basis set (aug-cc-pVDZ or aVDZ). For each isomer which is within 2 kcal mol^{-1} of the MP2/aVDZ global minimum, we do further geometric optimizations using very tight convergence criteria and calculate the harmonic vibrational calculations using ORCA.

The MP2 complete basis set limit (MP2/CBS) energy is estimated using explicitly correlated MP2-F12 method with cc-pVTZ-F12 orbital basis set along with cc-pVTZ- F12-CABS Complementary Auxiliary Basis Set (CABS) and cc-pVQZ/C auxiliary basis at the MP2/aVDZ optimized geometry. These methods are implemented in ORCA 4.2.1.[11] This method should fully be described as RI-MP2-F12/cc-pVTZ-F12//RI-MP2/aug-cc-pVDZ, however we will abbreviate it as MP2-F12/VTZ-F12//MP2/aVDZ in the rest of this manuscript for the sake of brevity.

These MP2-F12/VTZ-F12//MP2/aVDZ electronic energy (E_e) estimates are combined with the MP2/aVDZ harmonic zero-point and thermodynamic corrections to get zero-point corrected energies (E_0) and Gibbs free energies at finite temperatures [G(T)].

2.2 Rotational Constants, Principal Dipole Moments and Energies

2.2.1 $(CH_2F_2)_n$, where n = 2 − 4

The equilibrium theoretical rotational constants (A, B, C) and the principal dipole moment components (μ_a, μ_b, μ_c) are reported in the table below. The binding energy (ΔE_e, $\Delta E[0k]$, ΔG) for a cluster *k* is defined as the energy difference between the cluster (E_k) and its constituent monomers(E_1). The relative energy ($\Delta\Delta E_e$, $\Delta\Delta E[0k]$, $\Delta\Delta G$) for a cluster *k* is defined as the energy difference between the most stable cluster and cluster *k* (E_k).

$$\Delta E_k = E_k - n * E_1$$

$$\Delta\Delta E_k = E_k - \min_i\{E_i\}$$

The DFM clusters containing 2-4 monomers have already been studied by Prampolini et al.[12], but we have applied the above protocol to regenerate the structures and energies. The three most stable isomers for each cluster size are summarized in the table below.

Table S8. MP2/aVDZ rotational constants, principal dipole moments and MP2- F12/VTZ-F12//MP2/aVDZ relative energies of low energy isomers of $(CH_2F_2)_n$, where n = 2 − 4

	Rot. Consts (MHz)			Prin. Dipole Moment (Debye)				(kJ/mol)	
Label	A	B	C	μ_a	μb	μ_c	μ_{type}	ΔE_e	$\Delta\Delta E_e$
2-I	6162	1333	1278	2.64	-0.61	0.25	a	-12.3	0.0
2-II	12015	1004	938	0.00	0.00	0.00	-	-10.8	1.5
2-III	4516	1832	1435	0.00	0.01	0.00	-	-9.4	2.9
3-I	1386	840	622	-2.58	-0.76	-0.69	a	-27.2	0.0
3-II	1222	1002	703	0.78	1.14	0.46	b	-26.3	1.0
3-III	1256	797	552	2.03	-1.35	-0.13	a	-25.6	1.6
4-I	663	661	383	0.00	0.00	0.00	-	-45.7	0.0
4-II	840	499	372	0.00	0.00	0.00	-	-43.2	2.5
4-III	857	437	333	3.41	0.11	-0.52	a	-43.0	2.7

[a] Ordered by relative electronic energy (ΔΔE), with the global minimum labeled 'I', followed by 'II', 'III', 'IV' ... *etc* for higher energy isomers
[b] MP2-F12/VTZ-F12//MP2/aVDZ single point energies combined with thermodynamic corrections at MP2/aVDZ level of theory

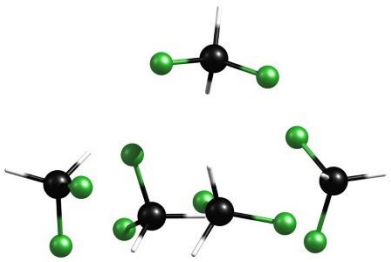
2.2.2 $(CH_2F_2)_5$

Pentamer data

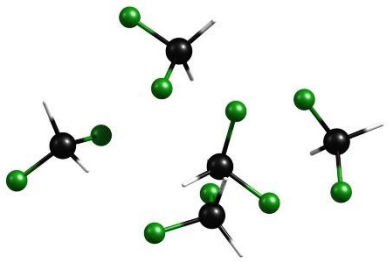
Table S9. MP2/aVDZ rotational constants, principal dipole moments and MP2- F12/VTZ-F12//MP2/aVDZ relative energies of low energy isomers of $(CH_2F_2)_n$, where n = 5

	Rot. Consts (MHz)			Prin. Dipole Moment (Debye)				(kJ/mol)	
Label	A	B	C	μ_a	μ_b	μ_c	μ_{type}	ΔE_e	$\Delta\Delta E_e$
5-I	441	375	292	0.2	-2.2	-0.9	b	-61.3	0.0
5-II	483	316	295	-3.1	0.4	-0.8	a	-61.0	0.3
5-III	495	331	231	1.4	-0.4	0.2	a	-60.8	0.4
5-IV	495	330	279	4.0	-0.1	-1.2	a	-60.3	1.0
5-V	461	350	281	0.5	1.1	-1.0		-60.2	1.0
5-VI	437	340	291	0.9	-0.5	1.9	c	-58.8	2.5
5-VII	426	351	270	-1.3	-1.3	-0.5		-56.3	5.0
Exp. 5-I	426.61950(7)	358.42855(5)	281.54415(5)	weak	strong	medium			

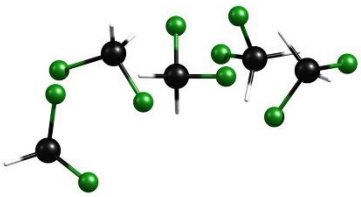
[a] Ordered by relative electronic energy ($\Delta\Delta E$), with the global minimum labeled 'I', followed by 'II', 'III', 'IV' ... *etc* for higher energy isomers
[b] MP2-F12/VTZ-F12//MP2/aVDZ single point energies combined with thermodynamic corrections at MP2/aVDZ level of theory



5-I



5-II



5-III

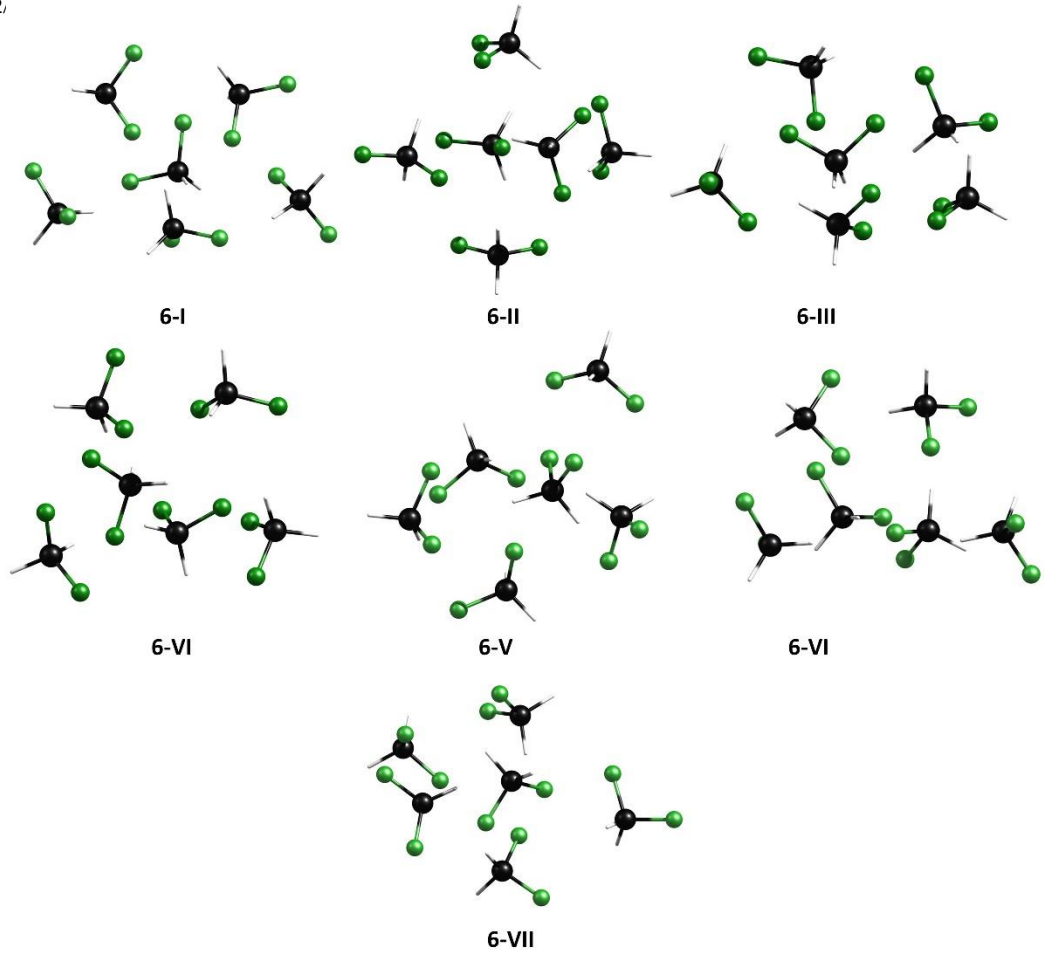
2.2.3 $(CH_2F_2)_6$

Hexamer data

Table S10. MP2/aVDZ rotational constants, principal dipole moments and MP2- F12/VTZ-F12//MP2/aVDZ relative energies of low energy isomers of $(CH_2F_2)_n$, where n = 6

	Rot. Consts (MHz)			Prin. Dipole Moment (Debye)				(kJ/mol)	
Label	A	B	C	μ_a	μb	μ_c	μ_{type}	ΔE_e	$\Delta\Delta E_e$
6-I	367	224	196	3.6	-0.8	-0.4	a	-79.6	0.0
6-II	324	277	237	-2.6	-0.8	-2.2		-79.2	0.4
6-III	363	232	214	-0.3	0.1	-1.1	c	-79.0	0.6
6-IV	312	281	229	-0.8	0.0	-0.6	a	-79.0	0.6
6-V	339	245	224	0.6	0.5	-2.2	c	-78.9	0.7
6-VI	372	226	190	3.7	-0.2	0.6	a	-78.9	0.7
6-VII	347	224	207	1.9	0.4	0.1	a	-78.8	0.8
6-VIII	291	266	243	2.4	2.3	-1.5		-78.6	1.0
6-IX	342	259	217	1.0	1.5	-0.9		-78.5	1.1
6-X	298	269	223	-2.0	0.9	0.2	a	-77.5	2.1
6-XI	362	230	210	0.8	-0.3	1.4	c	-76.7	2.7
Exp. 6-I	356.1116(7)	211.52526(4)	185.23390(5)	strong	weak	-			
Exp. 6-II	304.72043(7)	266.17778(5)	226.35912(5)	medium	-	weak			

[a] Ordered by relative electronic energy (ΔΔE), with the global minimum labeled 'I', followed by 'II', 'III', 'IV' ... *etc* for higher energy isomers
[b] MP2-F12/
of theory.



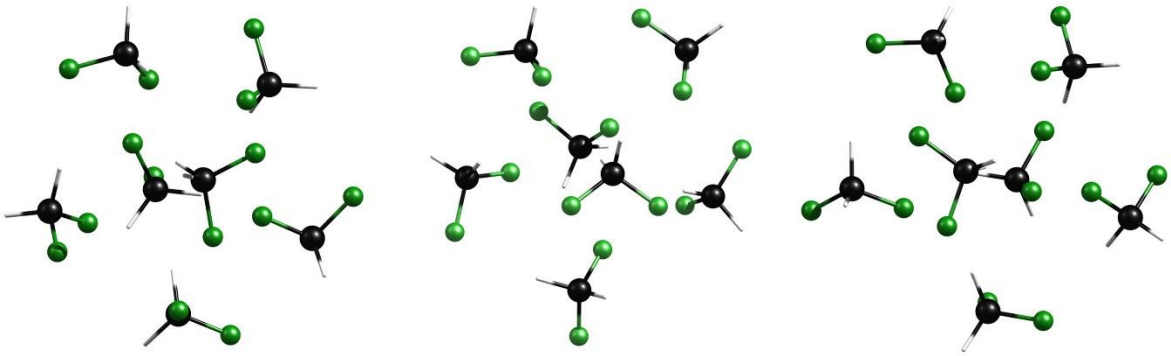
2.2.4 $(CH_2F_2)_7$

Heptamer data

Table S11. MP2/aVDZ rotational constants, principal dipole moments and MP2- F12/VTZ-F12//MP2/aVDZ relative energies of low energy isomers of $(CH_2F_2)_n$, where n = 7

	Rot. Consts (MHz)			Prin. Dipole Moment (Debye)				(kJ/mol)	
Label	A	B	C	μ_a	μb	μ_c	μ_{type}	ΔE_e	$\Delta\Delta E_e$
7-I	243	226	174	0.4	1.9	0.8	b	-99.5	0.0
7-II	233	222	162	-1.8	2.1	-0.5		-99.1	0.3
7-III	232	222	159	2.1	0.6	-1.2	a	-98.4	1.0
Exp. 7-II	229.5257(1)	215.0008(1)	163.3655(1)	medium	strong	weak			

[a] Ordered by relative electronic energy (ΔΔE), with the global minimum labeled 'I', followed by 'II', 'III', 'IV' ... *etc* for higher energy isomers
[b] MP2-F12/VTZ-F12//MP2/aVDZ single point energies combined with thermodynamic corrections at MP2/aVDZ level of theory



2.3 Many-Body Decomposition of Cluster Interaction Energies

2.3.1 Definition of Many-Body Decomposition

The total binding energy of a molecular cluster (E_{bind}) is often calculated in super-molecular approaches as the difference in energy between the cluster (E_c) and the N monomers constituting the cluster (E_m^i) in their isolated gas phase minimum geometries.

$$E_{bind} = E_c - \sum_i^N E_m^i$$

While binding energies calculated this way are meaningful, it is much more interesting to examine the energy associated with distortion of the monomers as they form a cluster, and the interactions between the monomers or groups thereof. When formulated that way, the binding energy is a sum of the monomer distortion energy (E_{dist}) and interaction energy (E_{int}) of a cluster.

$$E_{bind} = E_{dist} + E_{int}$$

The monomer distortion or relaxation energy (E_{dist}), which is also referred to as one-body energy (E_{1B}), is difference in energy between monomers in their isolated gas phase geometry (E_m^i) and cluster form (E_c^i)

$$E_{dist} = E_{iB} = \sum_i^N (E_c^i - E_m^i)$$

The interaction energy (E_{int}) can be expanded into its many-body components. The total interaction energy of a molecular cluster composed of N monomers is the sum of its two-body (2B), three-body (3B), four-body (4B), ... , N-body (NB) components.

$$E_{int} = E_{iB} + E_{2B} + E_{3B} + \ldots + E_{NB}$$

E_{2B} is the pair-wise interaction between all pairs of monomers in their cluster geometry.

$$E_{2B} = \sum_{i>j}^N \left[E_c^{ij} - \left(E_c^i + E_c^j\right)\right]$$

E_{3B} is the interaction between all sets of three monomers in their cluster geometry, excluding the 2B contribution.

$$E_{3B} = \sum_{i>j>k}^N \left[E_c^{ijk} - \left(E_c^i + E_c^j + E_c^k\right)\right] - E_{2B}$$

E_{4B} is the interaction between all sets of four monomers in their cluster geometry, excluding the smaller many-body contributions.

$$E_{4B} = \sum_{i>j>k>l}^{N} \left[E_c^{ijkl} - \left(E_c^i + E_c^j + E_c^k + E_c^l\right)\right] - E_{3B} - E_{2B}$$

and the general n-body contribution is

$$E_{\mathrm{n}B} = \sum_{i>j>\ldots n}^{N} \left[E_c^{ij\ldots n} - \left(E_c^i + E_c^j + \ldots + E_c^n\right)\right] - \sum_{a=2}^{n-1} [E_{aB}]$$

The monomer distortion or relaxation energy (E_{dist}, E_{iB}) is a generally positive quantity because monomers are adopting higher energy configurations with higher energies than in their isolated gas phase geometry in order to optimize their interactions with the other monomers constituting the cluster. Two-body interactions (E_{2B}) are the largest contributor to the stabilization of clusters, accounting for more than 80% of the total interaction energy in water clusters. Three-body interactions (E_{3B}) are also important especially in clusters composed of polar molecules where long-range forces are strong. E_{3B} generally accounts for 10-15% of the interaction energy in water clusters. Four- and other higher-body interactions may be non-negligible depending on the system and the desired level of accuracy.

For our purposes, many-body decomposition of the interaction energy provides insights into the strength of interactions between any pairs or triplets of monomers. Using a many-body decomposition code, we calculated all individual many-body interaction energy components between all sets of monomers to isolate different interactions.

Just to emphasize the subtle difference between the total interaction energy and binding energy, the two terms are defined below. Binding energy is the difference between the energy of the cluster and the energy of the isolated monomers in their minimum configuration. Interaction energy is the difference between the energy of the cluster and the energy of the isolated monomers in the cluster geometry. The difference between binding and interaction energy is the monomer distortion or relaxation energy (E_{dist}, E_{iB})

2.3.2 Definition of Cooperativity

Cooperativity in non-covalent interactions is an interesting phenomenon worth investigating. Positive cooperativity implies that the total interaction energy is greater than the sum of all pairwise interactions. Based on the definition of MBD terms above, the cooperativity energy (E_{coop}) would them be the sum of all n-body contributions past 2-body interactions:

$$E_{\mathrm{coop}} = E_{3B} + E_{4B} + E_{5B} + \ldots$$

$$E_{\mathrm{coop}} = \sum_{a=3}^{n-1} [E_{aB}]$$

2.3.3 $(CH_2F_2)_2$

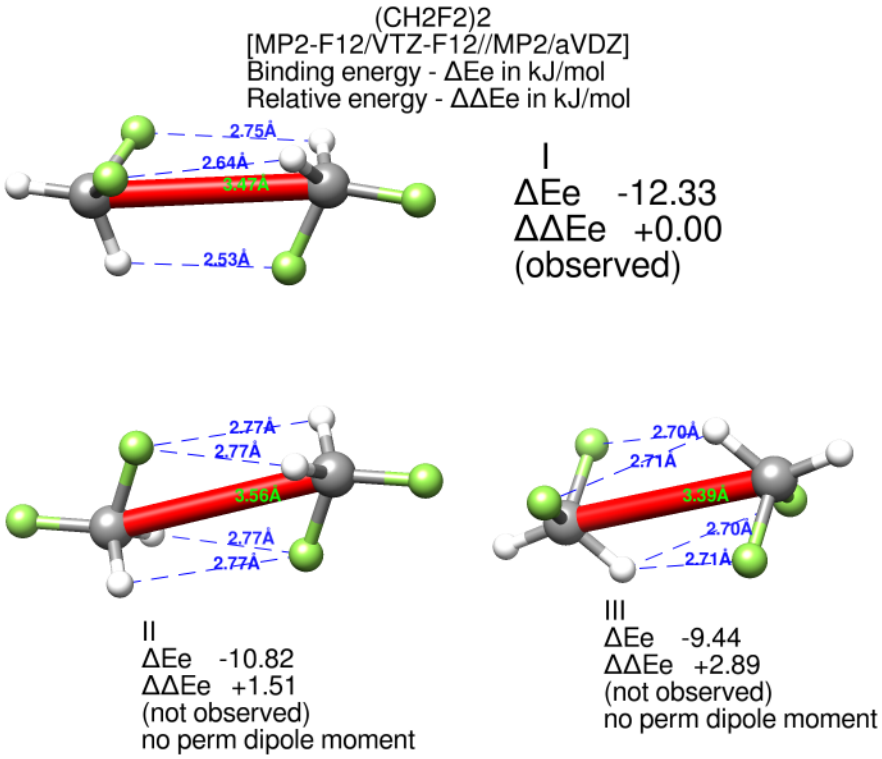


Figure S2. The three lowest energy isomers of $(CH_2F_2)_2$. The MBD of the interaction energy of (I) is reported in the table below.

Table S12. Many-body decomposition of the MP2-F12/VTZ-F12//MP2/aVDZ binding energy of $(CH_2F_2)_2$-I

All energies in kJ/mol	$(CH_2F_2)_2$-I
Individual 1-body contributions:	
Fragment 1(1) :	0.5
Fragment 2(2) :	0.5
Individual 2-body contributions:	
Fragment 1(1-2) :	-13.4
Many-body energies:	
1-body =	1.0
2-body =	-13.3
Interaction Energy =	-13.3
Binding Energy =	**-12.3**

2.3.4 $(CH_2F_2)_3$

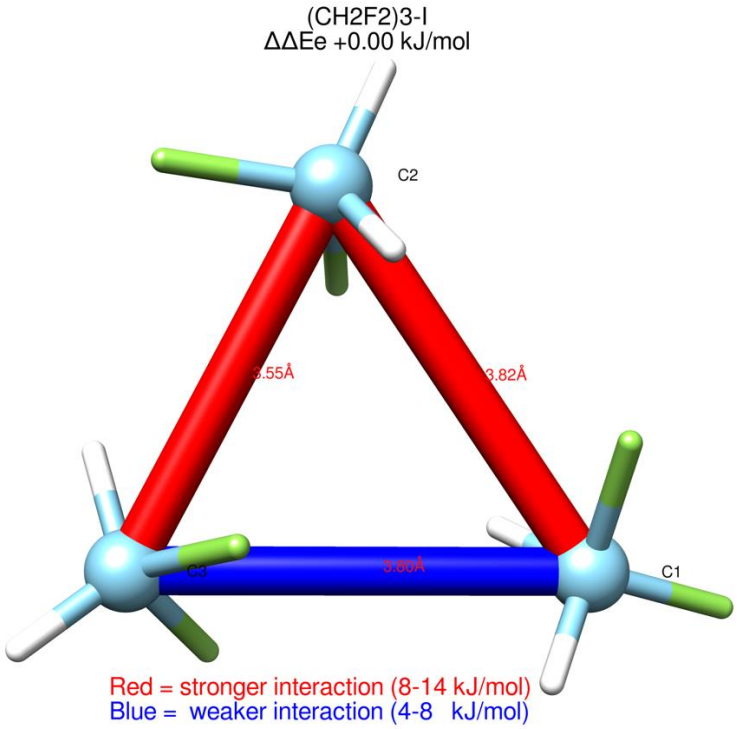


Figure S3.The lowest energy isomers of $(CH_2F_2)_3$. The carbon labels (C1,C2,C3) correspond to the monomer/fragment numbers in the table below.

Table 13. Many-body decomposition of the MP2-F12/VTZ-F12//MP2/aVDZ binding energy of $(CH_2F_2)_3$-I

	$(CH_2F_2)_3$-I
Individual 1-body contributions:	
Fragment 1(1) :	0.8
Fragment 2(2) :	1.0
Fragment 3(3) :	0.7
Individual 2-body contributions:	
Fragment 1(1-2) :	-10.3
Fragment 2(1-3) :	-7.4
Fragment 3(2-3) :	-11.4
Individual 3-body contributions:	
Fragment 1(1-2-3) :	-0.5
Many-body energies:	
1-body =	2.5
2-body =	-29.2
3-body =	-0.5
Interaction Energy =	-29.7
Binding Energy =	**-27.2**

2.3.5 $(CH_2F_2)_4$

Please note that the rotational spectrum of the two lowest energy isomers was not observed because they did not have a permanent dipole moment. Therefore, we report results for the observed isomer, $(CH_2F_2)_4$-III.

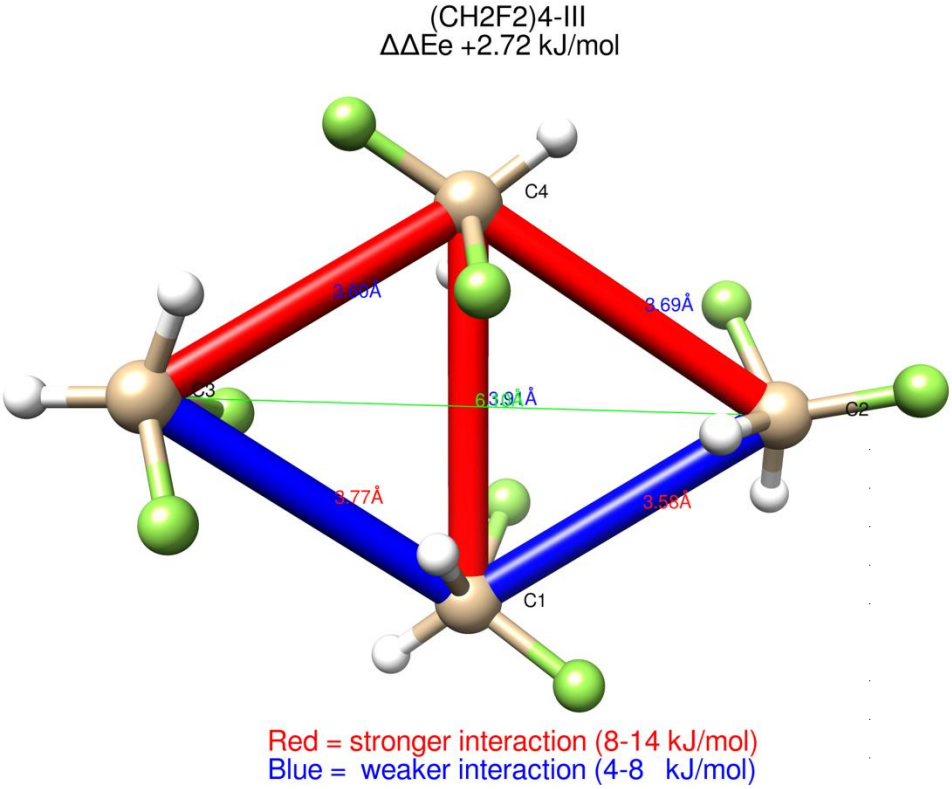


Figure S4. The third lowest energy isomer of $(CH_2F_2)_4$. The carbon labels (C1,C2, …) correspond to the monomer/fragment numbers in the table below.

Table S14. Many-body decomposition of the MP2-F12/VTZ-F12//MP2/aVDZ binding energy of $(CH_2F_2)_4$-III

	$(CH_2F_2)_4$-III
Individual 1-body contributions:	
Fragment 1(1) :	1.0
Fragment 2(2) :	0.6
Fragment 3(3) :	0.8
Fragment 4(4) :	1.5
Individual 2-body contributions:	
Fragment 1(1-2) :	-5.5
Fragment 2(1-3) :	-6.7
Fragment 3(1-4) :	-10.6
Fragment 4(2-3) :	-1.4
Fragment 5(2-4) :	-10.6
Fragment 6(3-4) :	-10.9
Individual 3-body contributions:	
Fragment 1(1-2-3) :	-0.7
Fragment 2(1-2-4) :	0.0
Fragment 3(1-3-4) :	-0.5
Fragment 4(2-3-4) :	0.0
Individual 4-body contributions:	
Fragment 1(1-2-3-4) :	-0.1
Many-body energies:	
1-body =	4.0
2-body =	-45.8
3-body =	-1.1
4-body =	-0.1
Interaction Energy =	-47.0
Binding Energy =	**-43.0**

2.3.6 $(CH_2F_2)_5$

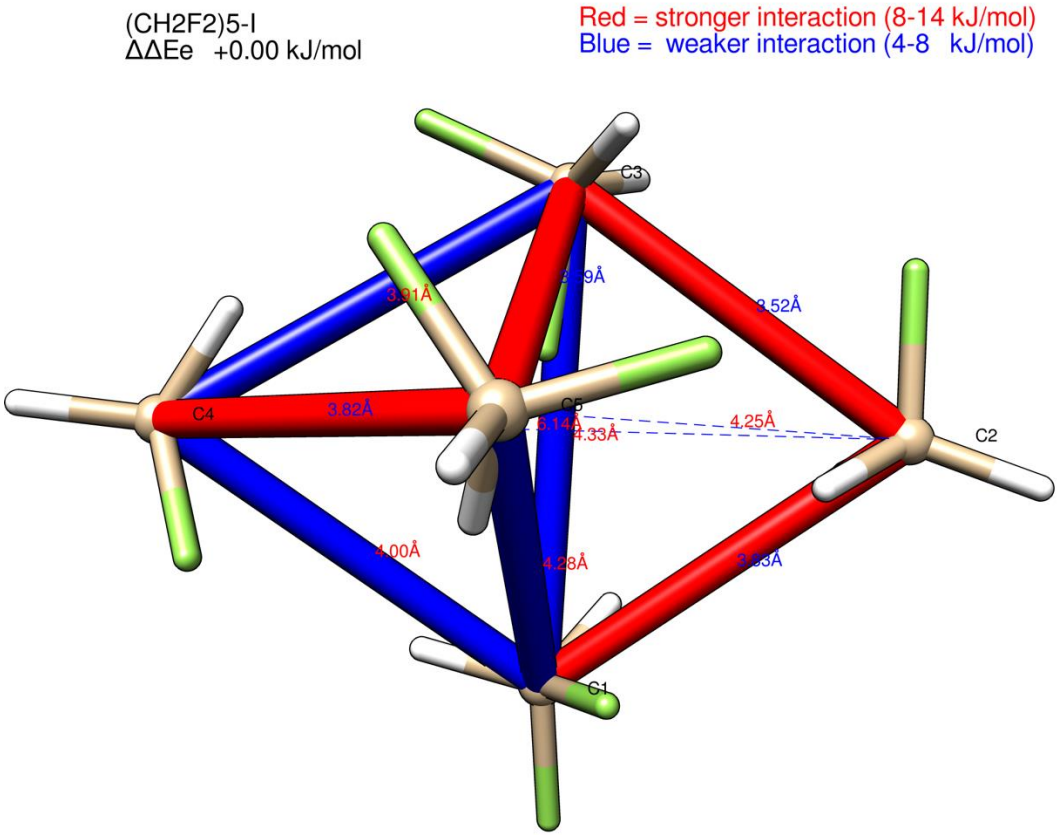


Figure S5.The lowest energy isomers of $(CH_2F_2)_5$. The carbon labels (C1,C2,C3) correspond to the monomer/fragment numbers in the table below.

Table S15. Many-body decomposition of the MP2-F12/VTZ-F12//MP2/aVDZ binding energy of $(CH_2F_2)_5$-I

	$(CH_2F_2)_5$-I
Individual 1-body contributions:	
Fragment 1(1) :	1.4
Fragment 2(2) :	1.0
Fragment 3(3) :	1.2
Fragment 4(4) :	1.0
Fragment 5(5) :	1.2
Individual 2-body contributions:	
Fragment 1(1-2) :	-10.6
Fragment 2(1-3) :	-5.4
Fragment 3(1-4) :	-5.8
Fragment 4(1-5) :	-4.3
Fragment 5(2-3) :	-10.8
Fragment 6(2-4) :	-0.8
Fragment 7(2-5) :	-1.8
Fragment 8(3-4) :	-5.1
Fragment 9(3-5) :	-10.9
Fragment 10(4-5) :	-10.8
Individual 3-body contributions:	
Fragment 1(1-2-3) :	-0.2
Fragment 2(1-2-4) :	0.0
Fragment 3(1-2-5) :	0.0
Fragment 4(1-3-4) :	0.2
Fragment 5(1-3-5) :	-0.5
Fragment 6(1-4-5) :	-0.4
Fragment 7(2-3-4) :	-0.3
Fragment 8(2-3-5) :	0.4
Fragment 9(2-4-5) :	0.1
Fragment 10(3-4-5) :	-0.2
Individual 4-body contributions:	0.0
Individual 5-body contributions:	0.0
Many-body energies:	
1-body =	5.8
2-body =	-66.2
3-body =	-0.9
4-body =	0.0
5-body =	0.0
Interaction Energy =	-67.1
Binding Energy =	**-61.3**

2.3.7 $(CH_2F_2)_6$

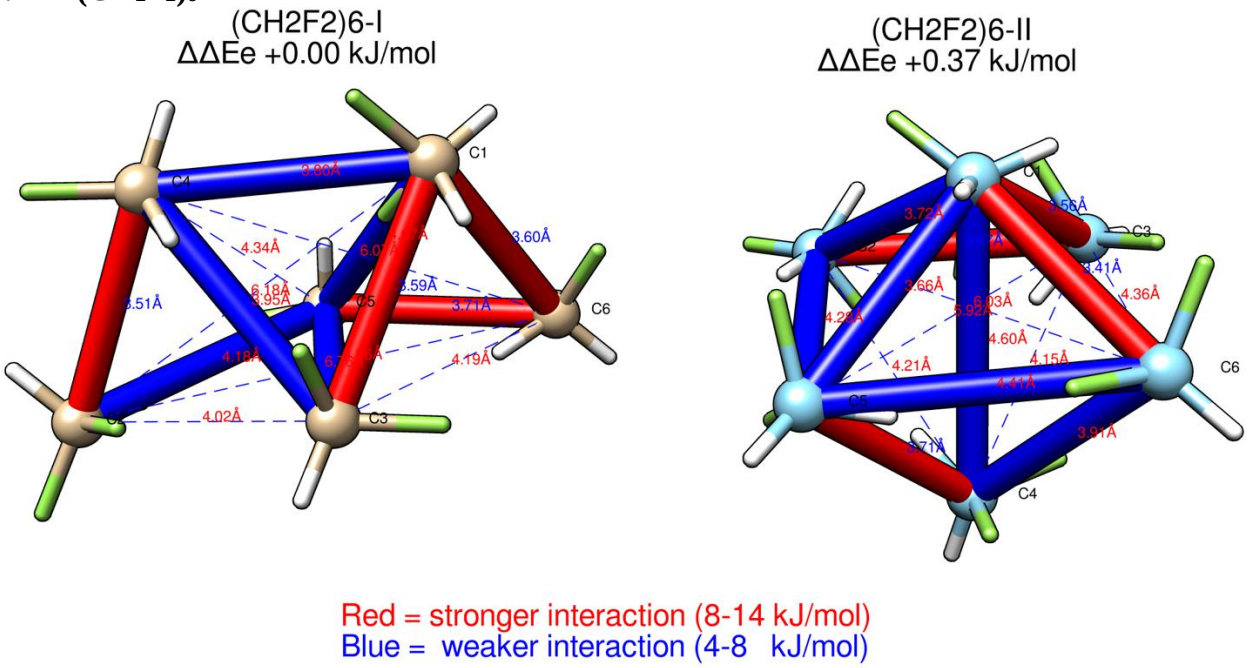


Figure S6.The two lowest energy isomers of $(CH_2F_2)_6$. The carbon labels (C1,C2,C3) correspond to the monomer/fragment numbers in the table below.

Table S16. Many-body decomposition of the MP2-F12/VTZ-F12//MP2/aVDZ binding energy of $(CH_2F_2)_6$-I and $(CH_2F_2)_6$-II

	$(CH_2F_2)_6$-I	$(CH_2F_2)_6$-II
Individual 1-body contributions:		
Fragment 1(1) :	1.2	1.7
Fragment 2(2) :	1.2	1.6
Fragment 3(3) :	1.4	0.9
Fragment 4(4) :	1.2	1.3
Fragment 5(5) :	1.2	1.0
Fragment 6(6) :	0.9	1.0
Individual 2-body contributions:		
Fragment 1(1, 2)	-1.2	-6.9
Fragment 2(1, 3)	-11.4	-10.9
Fragment 3(1, 4)	-5.8	-5.9
Fragment 4(1, 5)	-4.2	-4.2
Fragment 5(1, 6)	-9.3	-11.7
Fragment 6(2, 3)	-4.1	-10.7
Fragment 7(2, 4)	-13.3	-3.5
Fragment 8(2, 5)	-5.6	-6.2
Fragment 9(2, 6)	-0.7	-1.5
Fragment 10(3, 4)	-7.6	-1.8
Fragment 11(3, 5)	-5.6	-0.6
Fragment 12(3, 6)	-2.5	-1.2
Fragment 13(4, 5)	-2.5	-10.4
Fragment 14(4, 6)	-0.4	-6.4
Fragment 15(5, 6)	-11.6	-4.3
Individual 3-body contributions:	-1.0	-0.6
Individual 4-body contributions:	0.0	0.0
Individual 5-body contributions:	0.0	0.0
Individual 6-body contributions:	0.0	0.0
Many-body energies:		
1-body =	7.1	7.5
2-body =	-85.7	-86.1
3-body =	-1.0	-0.6
4-body =	0.0	0.0
5-body =	0.0	0.0
6-body =	0.0	0.0
Interaction Energy =	-86.7	-86.7
Binding Energy =	**-79.6**	**-79.2**

2.3.8 $(CH_2F_2)_7$

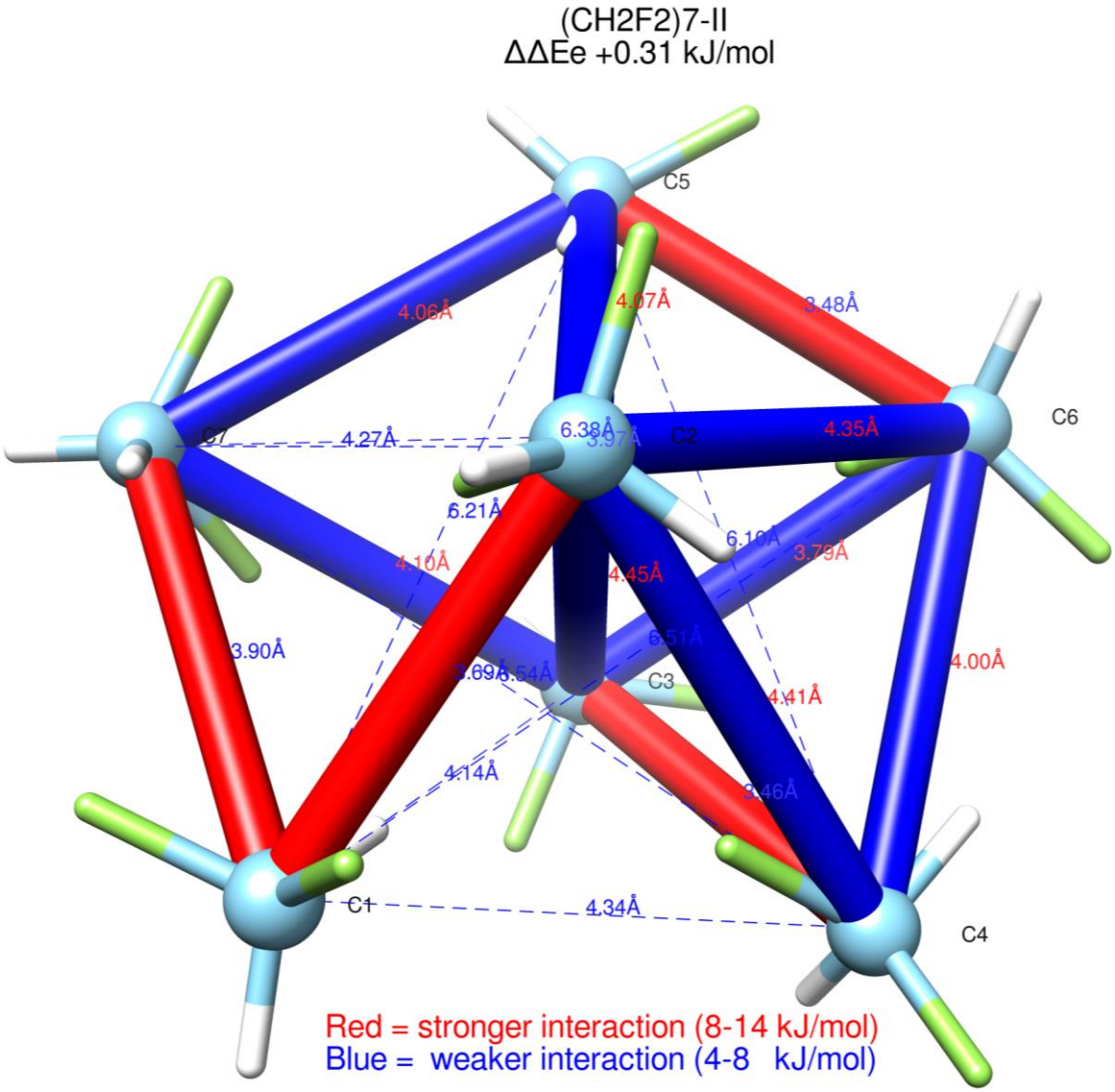


Figure S7.The lowest energy isomers of $(CH_2F_2)_7$. The carbon labels (C1,C2,C3) correspond to the monomer/fragment numbers in the table below.

Table S17. Many-body decomposition of the MP2-F12/VTZ-F12//MP2/aVDZ binding energy of $(CH_2F_2)_7$-II

	$(CH_2F_2)_7$-II
Individual 1-body contributions:	
Fragment 1(1) :	1.0
Fragment 2(2) :	1.5
Fragment 3(3) :	1.5
Fragment 4(4) :	1.2
Fragment 5(5) :	1.3
Fragment 6(6) :	1.1
Fragment 7(7) :	0.7
Individual 2-body contributions:	
Fragment 1(1, 2)	-9.7
Fragment 2(1, 3)	-3.7
Fragment 3(1, 4)	-2.5

Fragment 4(1, 5)	-1.0
Fragment 5(1, 6)	-0.8
Fragment 6(1, 7)	-9.9
Fragment 7(2, 3)	-6.2
Fragment 8(2, 4)	-5.1
Fragment 9(2, 5)	-6.8
Fragment 10(2, 6)	-5.2
Fragment 11(2, 7)	-1.5
Fragment 12(3, 4)	-11.6
Fragment 13(3, 5)	-2.8
Fragment 14(3, 6)	-6.4
Fragment 15(3, 7)	-6.4
Fragment 16(4, 5)	-1.9
Fragment 17(4, 6)	-4.2
Fragment 18(4, 7)	-1.0
Fragment 19(5, 6)	-13.2
Fragment 20(5, 7)	-4.9
Fragment 21(6, 7)	-0.7
Individual 3-body contributions:	-1.8
Individual 4-body contributions:	-0.1
Individual 5-body contributions:	0.0
Individual 6-body contributions:	0.0
Individual 7-body contributions:	0.0
Many-body energies:	
1-body =	7.1
2-body =	-85.7
3-body =	-1.0
4-body =	0.0
5-body =	0.0
6-body =	0.0
7-body =	0.0
Interaction Energy =	-107.5
Binding Energy =	**-99.1**

2.3.9 Comparison of MBD of $(CH_2F_2)_n$ and $(H_2O)_n$

The table below summarizes the breakdown of the total interaction energy into its many body components for all the observed clusters. **Figure S7** shows that virtually all the interaction energy in these clusters comes from pair-wise (two-body) interactions. Higher many-body interactions are essentially zero. These findings suggest that pairwise interactions between the different monomers in the clusters dictate the overall structure of the cluster. There are not higher-order effects that give the clusters distinct structural features.

Table S18. N-body contribution to the interaction energy as a fraction of the total interaction energy (E_nb/E_total)

	$(CH_2F_2)_{2\text{-}7}$ clusters								
nb	**2-I**	**3-I**	**4-III**	**4-I**	**5-I**	**6-I**	**6-II**	**7-II**	**7-I**
1b	-0.08	-0.09	-0.09	-0.09	-0.09	-0.09	-0.10	-0.08	-0.08
2b	1.08	1.07	1.07	1.09	1.08	1.08	1.09	1.07	1.07
3b		0.02	0.03	0.00	0.01	0.01	0.01	0.02	0.01
4b			0.00	0.00	0.00	0.00	0.00	0.00	0.00
5b					0.00	0.00	0.00	0.00	0.00
6b						0.00	0.00	0.00	0.00
7b								0.00	0.00

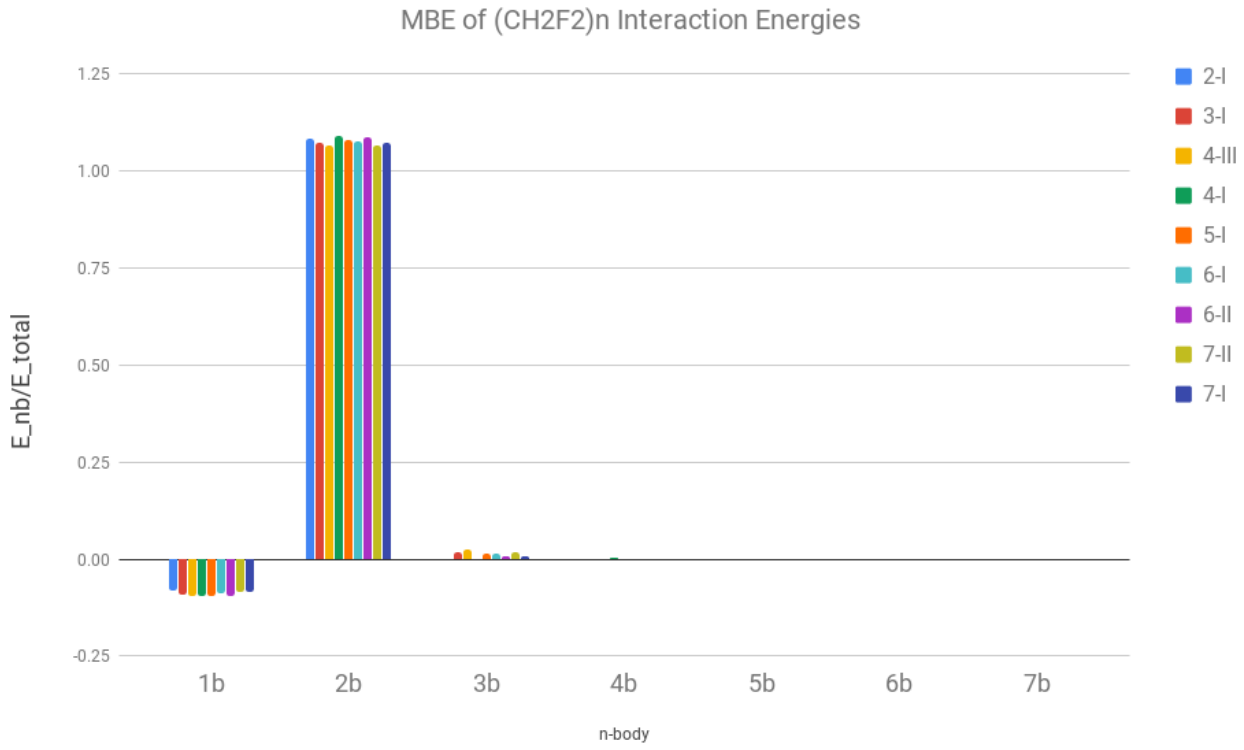


Figure S8. N-body contributions to the total interaction of $(CH_2F_2)_n$, n=2-7. 2-body interactions are dominant while larger N-body contributions are essentially zero.

The dominance of two-body interactions are in contrast to other systems like water clusters where three-body effects give the clusters their marked structural features.

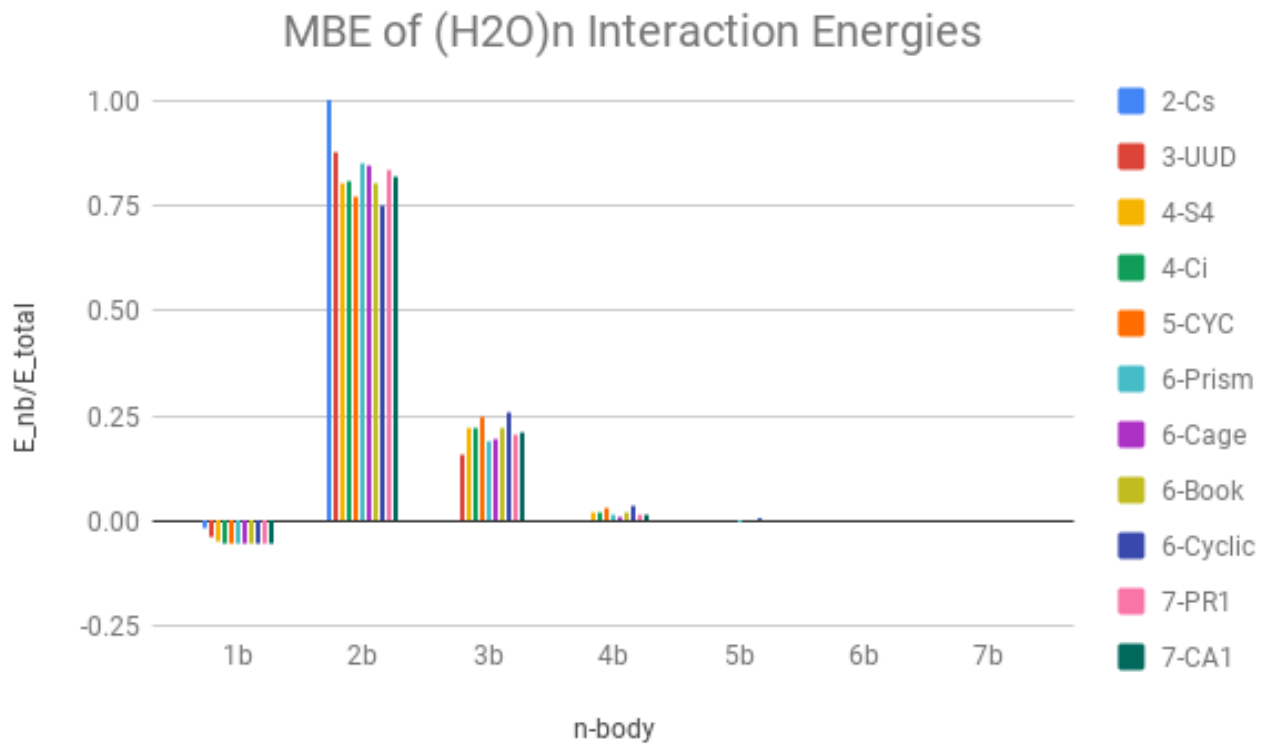


Figure S9. N-body contributions to the total interaction of $(H_2O)_n$, n=2-7. While 2-body interactions account for about 75% of the total interaction energy, 3-body interactions are significant (~20%) as well.

2.3.10 Distribution of two-body interaction energies and comparison with $(CH_2F_2)_2$

We have demonstrated that the interaction energy of difluoromethane clusters is largely dominated by pairwise (two-body) interactions. We can safely think of the clusters as a collection of dimers that distort to optimize their pair-wise interactions.

These constituent dimers span a large range in terms of geometry and binding energy. Some are very strongly bound, with structures and energies resembling that of an isolated dimer. These have two-body interaction energies (E_{2b}) close to that of the most stable isolated dimer (about -13 kJ/mol) or that of low energy stable (minima) and meta-stable (1^{st}-order transition states) (-8 to -13 kJ/mol). Others look like less stable dimers with E_{2b} of -4 to -8 kJ/mol, while the remaining have small attractive (0 to -4 kJ/mol) or even repulsive ($E_{2b} > 0$) interactions.

Figure S9 shows a histogram of the distribution of these two-body interaction energies in the $(CH_2F_2)_{n=2-7}$ clusters investigated in this study. It demonstrates that there are a set of strong ($-8 > E_{2b} > -13$), weak ($-4 > E_{2b} > -8$) and very weak ($E_{2b} > -4$) dimers.

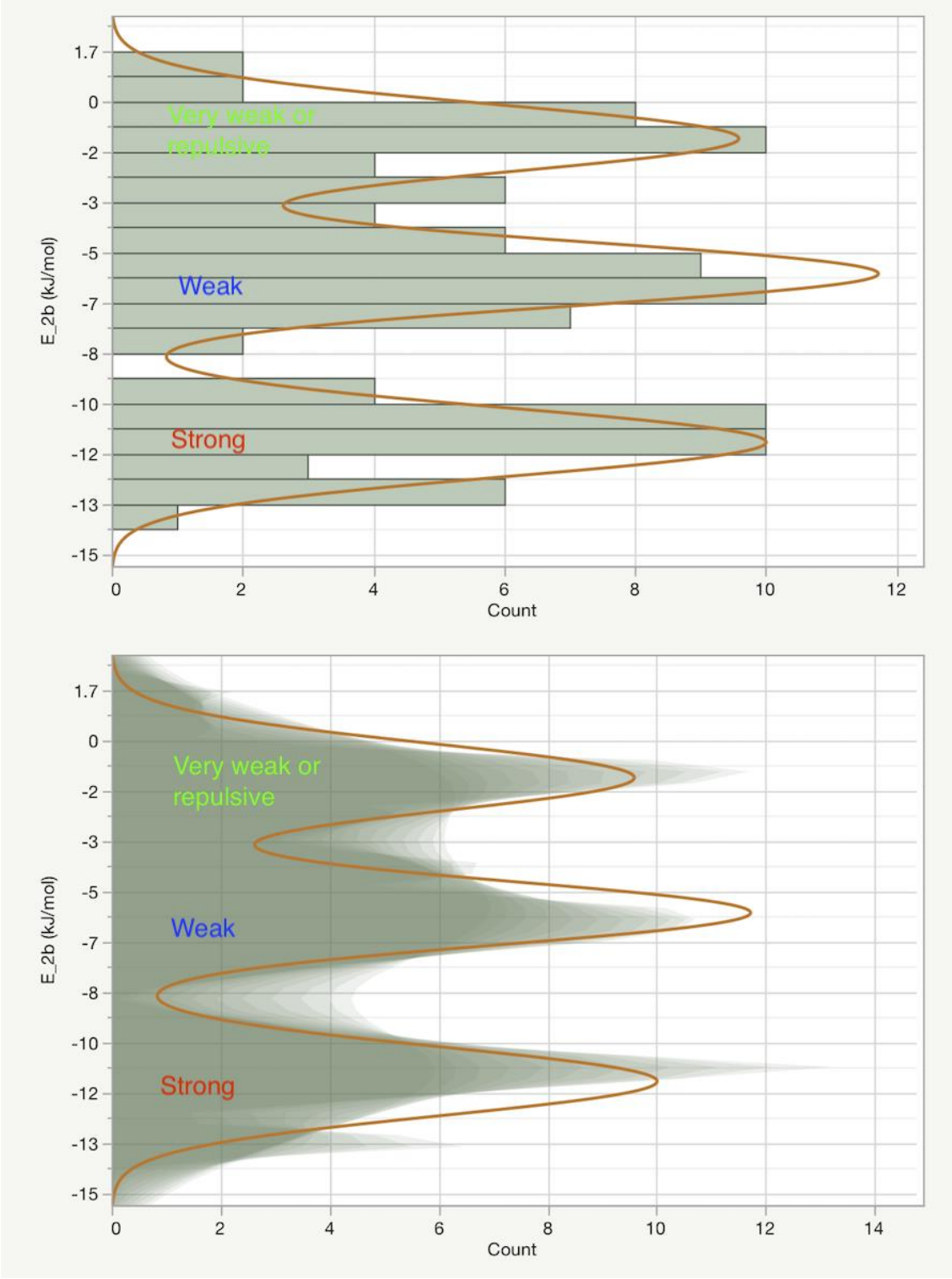


Figure S10. The distribution of the two-body interaction energies in the $(CH_2F_2)_{n=2-7}$ clusters investigated in this study. The figures show a histogram (top) or shadow histogram fitted to a sum of three normal distribution functions (bottom).

The two-body interaction energies of clusters are similar to those of isolated dimers, as shown in the figure below. Most of the isolated dimer isomers shown below are strongly bound although it is possible to find more weakly bound dimers if we search for higher-order transition states. Nevertheless, the presence of so many stable or metastable dimer building blocks leads to a vast number of conformers in larger clusters.

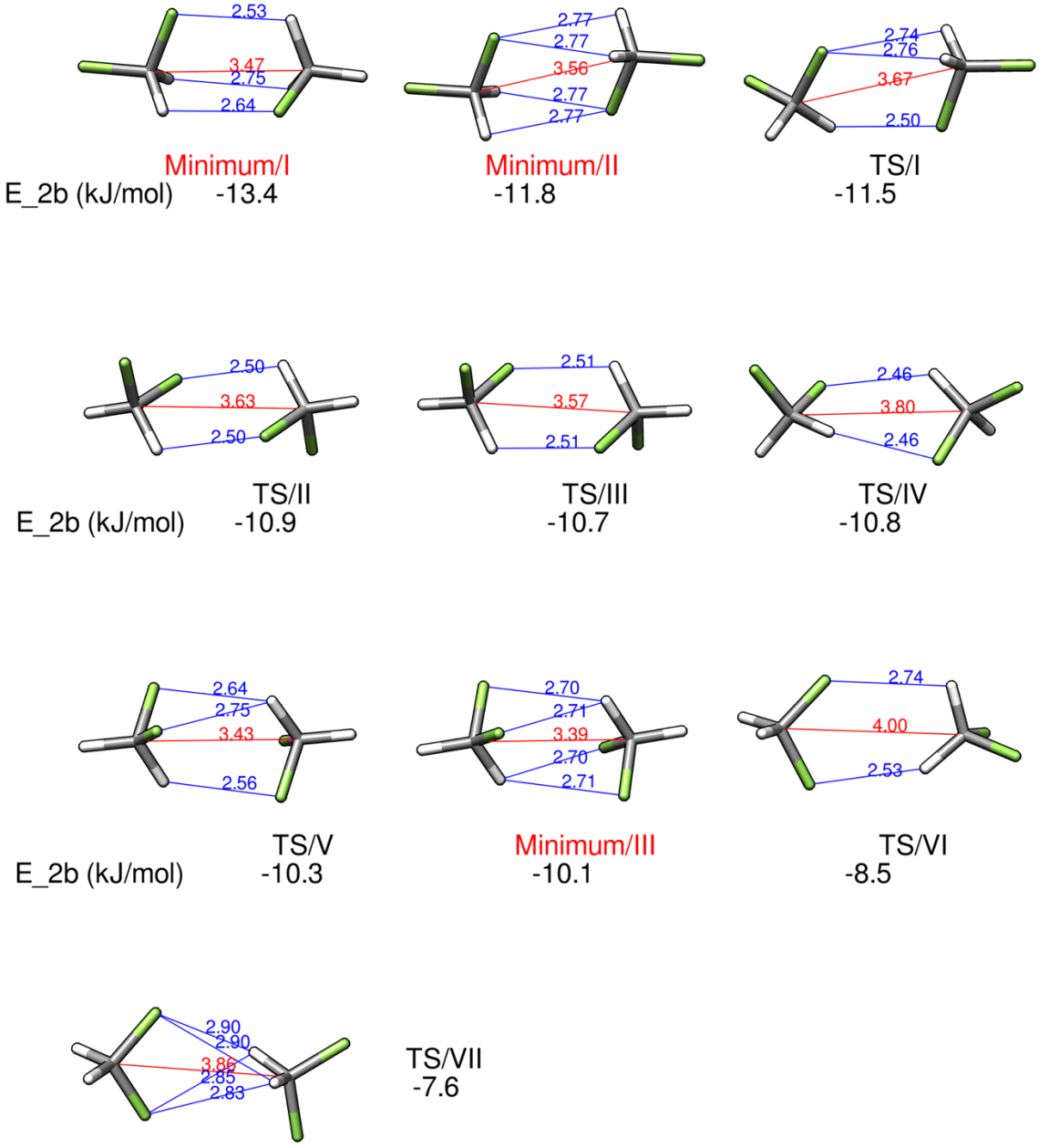


Figure S11. The interaction energy of many low energy minima and first-order transition states of difluoromethane dimer.

Therefore, we can think of these clusters as a set of monomers held together by pair-wise interactions. There are little higher-order, non-additive contributions that lead to particular structural motifs.

2.3.11 Takeaways from MBD Analysis

The many-body decomposition of the binding energy reported above leads to the following conclusions.

- **Monomer distortion:** Due to the limited degrees of freedom available to the DFM monomers, they undergo very small distortions relative to their isolated analogs. The distortion energy per monomer is usually 1-2 kJ/mol, which is comparable to water clusters.

- **Two-body interaction:** As mentioned in the previous section, these 2B interactions are what hold the clusters together. Each monomer distorts to optimize its pairwise interactions with its neighbors. The fact that the isolated dimer itself has a large number of low-energy isomers (see **Figure S10**) confers vast conformational flexibility to the larger clusters.

- **Three- and higher-body interactions:** Many-body interactions past two-body ones are negligible and they have little to no effect on the structures of the clusters.

- **Cooperativity:** the small three- and higher-body interaction energy contributions suggest that cooperative effects are present, but very small.

Therefore, we can think of these clusters as a set of monomers held together by pair-wise interactions. Higher-order, non-additive contributions are too small to lead to particular structural motifs.

2.4 Using SAPT to understand MBD Findings

One reason many-body contributions to the interaction energy of DFM clusters are very small relative to water clusters is due to the increased importance of dispersion in DFM clusters compared to prototypical hydrogen bonded systems like water clusters. Dispersion is less directional, therefore it allows for more disordered structures.

We can decompose the interaction energy of any dimer into its physically meaningful constituents (electrostatics, exchange repulsion, induction and dispersion) using symmetry-adapted perturbation theory (SAPT)[13,14] as implemented in PSI4[15] package. To understand the importance of these different constituents, we have chosen to compare DFM dimer with water dimer and methane dimer.

Table S19. SAPT2+3/aVDZ interaction energy components of three prototypical dimers

Dimers	Electrostatics	Exchange	Induction	Dispersion	Total
$(H_2O)_2$	-34.1	34.73	-10.38	-9.46	-19.25
$(CH_2F_2)_2$	-15.15	15.23	-2.43	-10.67	-13.01
$(CH_4)_2$	-1.26	4.39	-0.21	-4.81	-1.88

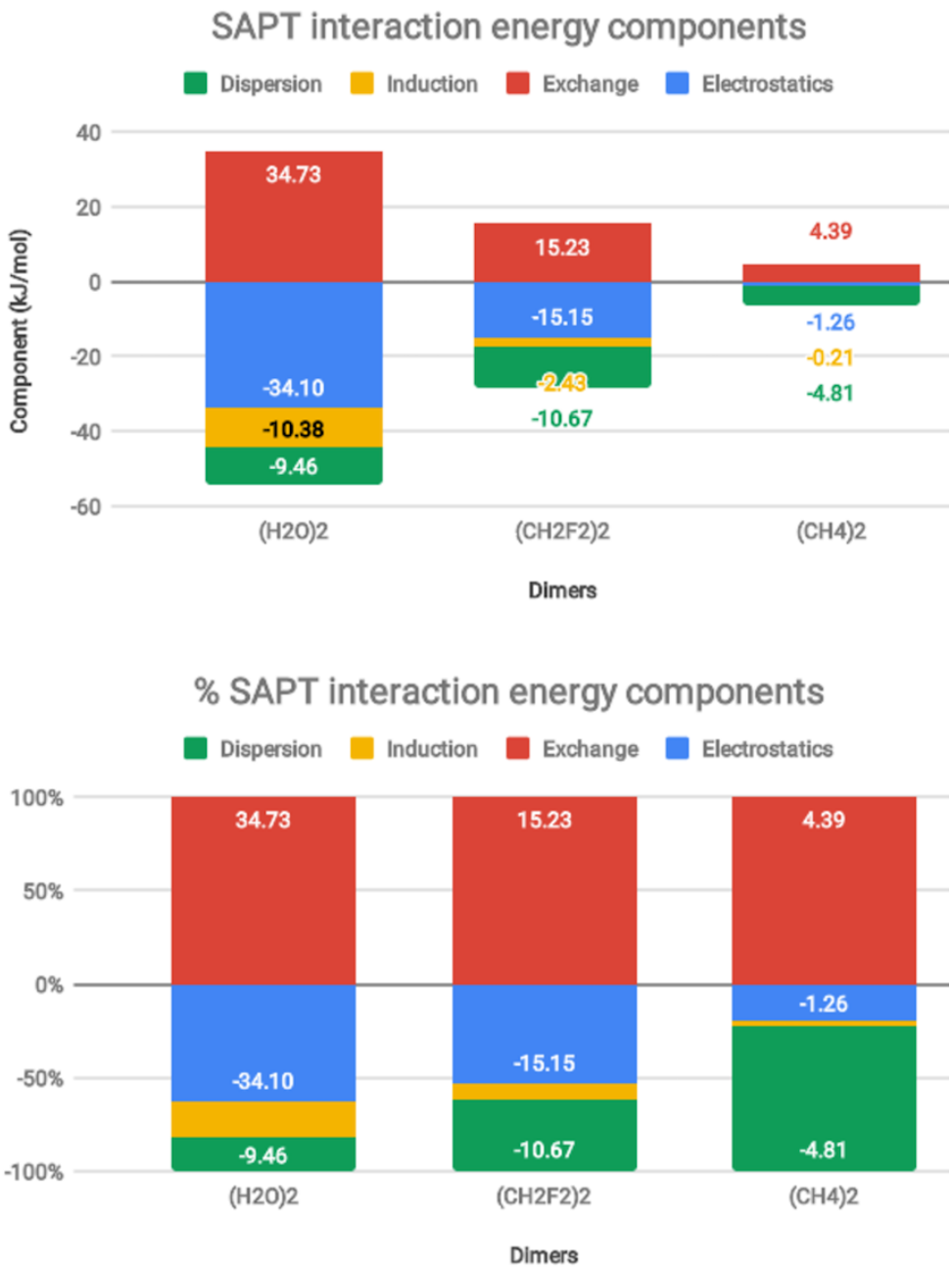


Figure S12. SAPT2+3/aVDZ interaction energy components (top) as a percentage of the total interaction energy (bottom)

As **Table S19** and **Figure S13** show, the total magnitude and constituent components of the interaction energy differ a lot in these three dimers.

- Water dimer is held together by a strong hydrogen bond (~20 kJ mol^{-1}). Due to water monomer's permanent dipole moment and the lone pairs on the oxygens, all three attractive components (electrostatics, induction and dispersion) of the SAPT interaction energy are important. The electrostatic component cancels out exchange repulsion and that leaves induction and dispersion as the remaining attractive components.
- DFM dimer is held together by a number of weak hydrogen bonds (two ~6 kJ mol^{-1} or three ~4 kJ mol^{-1} or four ~3 kJ mol^{-1}). While it has a permanent dipole and large electron density around the fluorine, the electrostatic component in DFM dimer is about half that of water dimer. The

electrostatic component here is cancelled out by exchange repulsion of the same magnitude, leaving induction and dispersion as the main forces holding the dimer together. The dispersion component in DFM dimer is in fact larger than that of water dimer. The increased importance of dispersion leads to less directional interaction and more disordered structures.

- Methane dimer is largely held together by dispersion interactions because the monomers do not have permanent dipole moment. The absence of a strongly directional interaction means the shapes they form are mainly a function of steric repulsion and dispersive attraction.

Therefore, the progressively larger role dispersion plays in the total interaction energy as one goes from water dimer to DFM dimer to methane dimer correlates with the increasingly disordered structure of the larger clusters.

2.5 Cartesian Coordinates

2.5.1 CH_2F_2 monomer

Cartesian coordinates of the DFM monomer and observed clusters is provided below in Angstrom units.

Table S20. MP2/aVDZ optimized Cartesian coordinates of DFM (CH_2F_2) monomer

5			
Monomer			
F	2.2235	1.1410	-1.0907
F	3.4390	0.9691	0.7724
C	3.1619	0.3727	-0.4378
H	4.0805	0.3584	-1.0385
H	2.7304	-0.6186	-0.2479

2.5.2 $(CH_2F_2)_2$

Table S21. MP2/aVDZ optimized Cartesian coordinates of $(CH_2F_2)_2$

10			
Dimer-I(observed)			
C	-1.49129	-0.52627	0.06876
H	-1.39502	-0.85984	1.10855
H	-1.05131	-1.20707	-0.66905
F	-0.87114	0.70524	-0.05183
F	-2.82640	-0.35406	-0.22205
C	1.97096	-0.47371	0.16271
H	3.05028	-0.62115	0.29030
H	1.65465	0.57136	0.07312
F	1.32254	-1.03762	1.24418
F	1.56635	-1.15487	-0.96698

2.5.3 $(CH_2F_2)_3$

Table S22. MP2/aVDZ optimized Cartesian coordinates of $(CH_2F_2)_3$

15			
Trimer-I(observed)			
F	0.346241	2.310068	-0.035071
F	-1.250138	3.727727	-0.676258
C	-0.957754	2.392970	-0.497220
H	-1.624152	1.981371	0.267631
H	-1.011727	1.885838	-1.467333
F	-1.011318	0.625365	2.306962
F	0.262312	-1.189537	2.516957
C	0.299178	0.181745	2.349952
H	0.784149	0.626044	3.227324
H	0.774403	0.411213	1.391777
F	-0.709021	-0.674775	-0.441241
F	-2.907288	-0.349489	-0.281818
C	-1.897991	-1.257444	-0.038444
H	-1.844301	-1.448729	1.038319
H	-2.072032	-2.146279	-0.657024

2.5.4 $(CH_2F_2)_4$

Table S23. MP2/aVDZ optimized Cartesian coordinates of $(CH_2F_2)_4$

20			
Tetramer-III(observed)			
C	-0.11610	1.97410	0.32100
H	-0.83260	2.64210	0.81200
H	-0.53550	1.37590	-0.49260
F	0.41190	1.12010	1.27420
F	0.93030	2.73050	-0.17270
C	2.86360	0.04030	-0.15170
H	3.05820	0.90500	0.49170
H	2.04130	0.17830	-0.86270
F	2.56610	-1.04750	0.65300
F	4.00880	-0.26420	-0.85380
C	-3.23670	-0.03830	-0.32760
H	-2.89670	-0.97700	-0.77630
H	-4.30580	-0.00190	-0.08590
F	-2.94800	1.00060	-1.19090
F	-2.51980	0.17860	0.83530
C	-0.23260	-1.93130	0.26970
H	-0.22350	-1.31680	1.17500
H	0.61030	-2.62190	0.16870
F	-0.23860	-1.08480	-0.83080
F	-1.40870	-2.65710	0.22860

2.5.5 $(CH_2F_2)_5$

Table S24. MP2/aVDZ optimized Cartesian coordinates of $(CH_2F_2)_5$-I

25			
Pentamer-I(observed)			
F	8.74518	-11.41164	-0.01849
F	7.49198	-9.74584	-0.81100
C	7.86381	-10.42039	0.34921
H	8.37567	-9.71110	1.00703
H	6.96567	-10.88135	0.77325
F	4.61106	-11.17463	0.11047
F	3.21436	-9.47115	-0.22722
C	4.22388	-10.21759	-0.80889
H	5.07330	-9.56018	-1.01311
H	3.81067	-10.72916	-1.68632
F	5.06227	-7.19180	2.93084
F	5.76452	-8.53165	1.29413
C	4.63422	-7.97904	1.88111
H	4.02176	-8.79547	2.27815
H	4.13674	-7.34605	1.14014
F	8.49929	-8.21144	3.00157
F	8.85555	-7.18242	1.05821
C	8.39219	-6.99903	2.35239
H	9.05096	-6.27816	2.85139
H	7.33812	-6.71138	2.30919
F	5.23404	-7.11250	-1.35479
F	6.14985	-5.82442	0.21730
C	6.43276	-6.59008	-0.90038
H	7.08736	-7.41463	-0.60834
H	6.83581	-5.92799	-1.67585

2.5.6 $(CH_2F_2)_6$

Table S25. MP2/aVDZ optimized Cartesian coordinates of $(CH_2F_2)_6$-I

30			
Hexamer-I(observed)			
F	1.34150	0.83650	-0.59240
F	1.26840	3.03510	-0.93840
C	2.05290	2.01750	-0.43500
H	2.96820	1.94880	-1.03200
H	2.21010	2.18500	0.63550
F	-2.72930	0.08960	1.15770
F	-4.15390	-1.62450	1.20380
C	-3.34880	-0.87640	0.37340
H	-2.57660	-1.52340	-0.05500
H	-3.97570	-0.36180	-0.36330
F	1.31430	0.36830	2.47640
F	-0.16950	1.87120	1.76960
C	-0.01270	0.53950	2.10750
H	-0.64480	0.32380	2.97530
H	-0.21200	-0.07690	1.22830
F	-1.41090	0.33150	-1.50650
F	-2.98120	1.90880	-1.51500
C	-1.63540	1.68630	-1.30550
H	-1.06420	2.24470	-2.05470
H	-1.39090	1.93110	-0.26770
F	0.27320	-2.07700	0.12890
F	-1.00440	-2.62210	-1.61220
C	0.26330	-2.21620	-1.25360
H	0.97460	-3.00420	-1.52230
H	0.46630	-1.23800	-1.69950
F	4.08410	-0.00340	0.29650
F	3.18490	-1.70460	-0.83220
C	3.40710	-1.20110	0.43640
H	2.44320	-1.00490	0.91310
H	2.44320	-1.00490	0.91310
H	4.05680	-1.90110	0.97530

Table S26. MP2/aVDZ optimized Cartesian coordinates of $(CH_2F_2)_6$-II

30			
Hexamer-II(observed)			
F	0.19430	-0.25060	0.57220
F	-0.14720	-0.64050	2.74200
C	0.80360	-0.68710	1.74950
H	1.61080	0.01160	1.98860
H	1.11470	-1.72610	1.60150
F	-3.85060	1.16210	1.54980
F	-2.23370	1.51780	0.05670
C	-2.55490	0.82970	1.22580
H	-2.50140	-0.24330	1.01550
H	-1.88490	1.17690	2.01870
F	2.01450	2.10650	0.47630
F	0.38800	2.38330	1.97590
C	0.78850	2.70770	0.69190
H	0.06440	2.29570	-0.01510
H	0.92300	3.79460	0.63770
F	0.11400	-0.70950	-2.83220
F	0.31450	1.43460	-2.26080
C	-0.60350	0.42150	-2.48500
H	-1.14800	0.22810	-1.55800
H	-1.23140	0.70810	-3.33660
F	-2.13570	-1.86300	-0.85110
F	-1.03020	-2.95090	0.75170
C	-1.09450	-2.74700	-0.61130
H	-0.16030	-2.28810	-0.94700
H	-1.34060	-3.70030	-1.09410
F	3.50080	-0.59250	0.18870
F	2.17400	-1.98760	-0.92680
C	2.81940	-0.76260	-0.99920
H	3.54740	-0.80840	-1.81750
H	2.07040	0.02850	-1.09400

2.5.7 $(CH_2F_2)_7$

Table S27. MP2/aVDZ optimized Cartesian coordinates of $(CH_2F_2)_7$-II

35			
Heptamer-II(observed)			
F	-0.28813	-3.25292	1.40896
F	-2.06494	-3.39518	0.07282
C	-0.68255	-3.30769	0.08631
H	-0.27571	-4.22428	-0.35659
H	-0.38117	-2.38561	-0.41696
F	-0.96994	-0.40566	1.10835
F	-0.64856	0.77516	2.96807
C	-0.33453	-0.41466	2.34645
H	0.74444	-0.46125	2.17408
H	-0.74761	-1.24178	2.93252
F	0.51387	-1.21592	-2.42158
F	1.56984	0.73006	-2.17236
C	0.34307	0.09984	-2.02330
H	0.06874	0.11805	-0.96679
H	-0.37722	0.57693	-2.69407
F	1.84333	-1.44107	0.24513
F	4.00510	-1.98213	0.30530
C	3.08038	-1.18579	-0.33416
H	3.32995	-0.13425	-0.16077
H	3.02777	-1.47846	-1.38848
F	-0.70997	3.86928	0.74012
F	-0.96322	2.60646	-1.07579
C	-1.46565	2.84716	0.19348
H	-2.49988	3.19343	0.09422
H	-1.33591	1.94771	0.80021
F	3.33273	2.24893	0.20541
F	1.29285	1.50823	0.70909
C	2.00331	2.61694	0.27626
H	1.65367	2.87955	-0.72690
H	1.89567	3.40806	1.02574
F	-3.57877	0.70713	-0.24024
F	-2.38514	-0.70634	-1.48458
C	-3.42892	-0.62389	-0.58422
H	-4.34521	-0.95631	-1.08639
H	-3.16348	-1.19345	0.31071

2.6 Quantitative analysis for difluoromethane tetramer

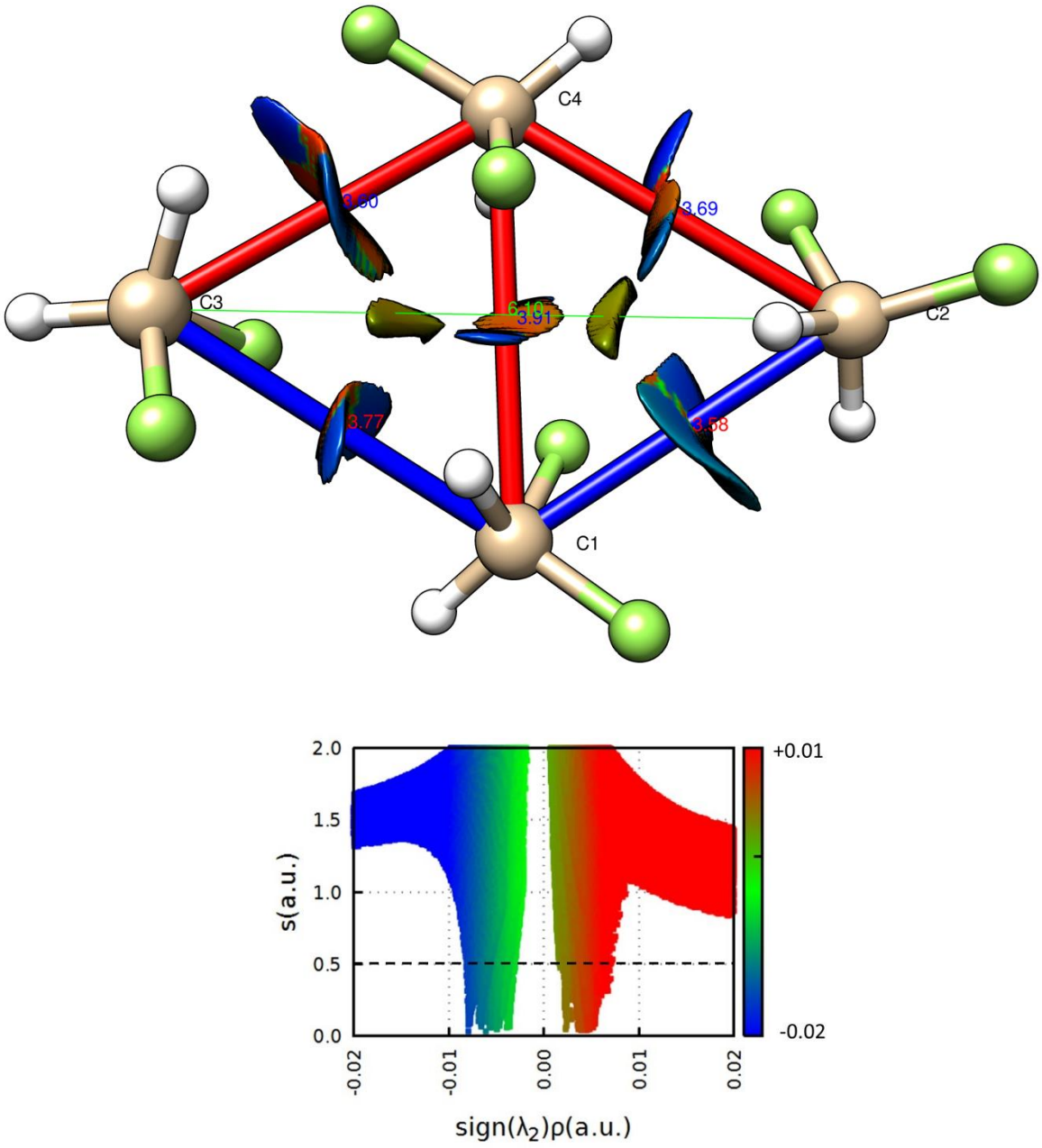


Figure S13. Quantitative analysis of attractive and repulsive interactions using the QTAIM procedure and NCI iso-surfaces. The carbon-carbon interaction distances are also reported. Blue- and green-colored areas indicate the presence of strong and weak attractive interactions, respectively. Red color signifies repulsive interactions. Bond-critical-point (BCP) paths are represented as blue lines. The iso-surface of the NCI analysis was build using s=0.5 and a blue-green-red color scale from $-0.02 < \text{sign}(\lambda_2)\,\rho(r) < +0.01$ a.u.

References

[1] G. G. Brown, B. C. Dian, K. O. Douglass, S. M. Geyer, S. T. Shipman, B. H. Pate, *Rev. Sci. Instrum.* **2008**, *79*, 053103.

[2] C. Pérez, S. Lobsiger, N. A. Seifert, D. P. Zaleski, B. Temelso, G. C. Shields, Z. Kisiel, B. H. Pate, *Chem. Phys. Lett.* **2013**, *571*, 1–15.

[3] I. Uriarte, C. Pérez, E. Caballero-Mancebo, F. J. Basterretxea, A. Lesarri, J. A. Fernández, E. J. Cocinero, *Chem. - A Eur. J.* **2017**, *23*, 7156.

[4] J. K. G. Watson, *Vibrational Spectra and Structure*, Elsevier Science Publishers, New York, Amsterdam, **1977**.

[5] T. T. Odbadrakh, A. G. Gale, B. T. Ball, B. Temelso, G. C. Shields, *J. Vis. Exp.* **2020**, *158*, e60964.

[6] D. E. Goldberg, *Genetic Algorithms in Search, Optimization and Machine Learning*, Addison-Wesley Longman Publishing Co., Inc., USA, **1989**.

[7] J. M. Dieterich, B. Hartke, *Mol. Phys.* **2010**, *108*, 279–291.

[8] J. J. P. Stewart, *J. Mol. Model.* **2013**, *19*, 1–32.

[9] J. J. P. Stewart, *MOPAC* **2008**.

[10] R. Sure, S. Grimme, *J. Comput. Chem.* **2013**, *34*, 1672–1685.

[11] F. Neese, *WIREs Comput. Mol. Sci.* **2018**, *8*, e1327.

[12] G. Prampolini, L. Carbonaro, G. Feng, L. Evangelisti, W. Caminati, I. Cacelli, *J. Chem. Theory Comput.* **2014**, *10*, 2204–2211.

[13] K. Szalewicz, *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2*, 254–272.

[14] T. M. Parker, L. A. Burns, R. M. Parrish, A. G. Ryno, C. D. Sherrill, *J. Chem. Phys.* **2014**, *140*, 16.

[15] J. M. Turney, A. C. Simmonett, R. M. Parrish, E. G. Hohenstein, F. A. Evangelista, J. T. Fermann, B. J. Mintz, L. A. Burns, J. J. Wilke, M. L. Abrams, N. J. Russ, M. L. Leininger, C. L. Janssen, E. T. Seidl, W. D. Allen, H. F. Schaefer, R. A. King, E. F. Valeev, C. D. Sherrill, T. D. Crawford, *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2*, 556–565.

Pentamer - 5 I

							obs	o-c	error	blends o-c	blends wt	Notes
1:	3	1	2	2	0	2	2261.5707	-0.0013	0.025			
2:	4	0	4	3	1	3	2352.8413	-0.0010	0.025			
3:	4	1	4	3	1	3	2355.0441	-0.0011	0.025			
4:	4	0	4	3	0	3	2361.7401	0.0001	0.025			
5:	4	1	4	3	0	3	2363.9425	-0.0004	0.025			
6:	3	3	1	2	2	0	2434.9927	-0.0003	0.025			
7:	3	3	0	2	2	0	2448.6892	-0.0017	0.025			
8:	3	3	1	2	2	1	2473.1529	-0.0013	0.025			
9:	4	1	3	3	2	2	2473.9902	-0.0004	0.025			
10:	3	3	0	2	2	1	2486.8511	-0.0010	0.025			
11:	4	2	3	3	2	2	2528.3062	-0.0048	0.025			
12:	4	1	3	3	1	2	2597.0208	-0.0007	0.025			
13:	4	3	2	3	3	1	2610.9127	-0.0158	0.025			
14:	4	2	3	3	1	2	2651.3416	-0.0003	0.025			
15:	4	2	2	3	2	1	2722.4107	0.0109	0.025			
16:	5	0	5	4	1	4	2919.9260	-0.0024	0.025			
17:	5	1	5	4	1	4	2920.4186	0.0000	0.025			
18:	5	0	5	4	0	4	2922.1294	-0.0019	0.025			
19:	5	1	5	4	0	4	2922.6201	-0.0013	0.025			
20:	4	2	2	3	1	2	2998.4237	-0.0015	0.025			
21:	4	3	2	3	2	1	3011.1796	0.0004	0.025			
22:	4	1	3	3	0	3	3053.5157	-0.0041	0.025			
23:	5	2	3	4	3	2	3078.0233	0.0054	0.025			
24:	4	3	1	3	2	1	3090.4225	-0.0021	0.025			
25:	5	1	4	4	2	3	3098.7966	-0.0015	0.025			
26:	5	1	4	4	1	3	3153.1164	-0.0021	0.025			
27:	4	3	2	3	2	2	3164.1718	-0.0020	0.025			
28:	5	2	4	4	1	3	3171.2179	-0.0010	0.025			
29:	4	3	1	3	2	2	3243.4176	-0.0016	0.025			
30:	5	3	3	4	3	2	3247.1477	-0.0012	0.025			
31:	4	4	1	3	3	0	3304.0698	-0.0019	0.025			
32:	4	4	0	3	3	0	3308.1062	-0.0016	0.025			
33:	4	4	1	3	3	1	3317.7690	-0.0007	0.025			
34:	4	4	0	3	3	1	3321.8045	-0.0013	0.025			
35:	5	2	3	4	2	2	3366.7963	-0.0008	0.025			
36:	5	3	2	4	3	1	3397.7755	-0.0023	0.025			
37:	4	2	2	3	1	3	3446.0384	0.0124	0.025			
38:	6	0	6	5	1	5	3483.9435	-0.0019	0.025			
39:	6	1	6	5	1	5	3484.0450	-0.0026	0.025			
40:	6	0	6	5	0	5	3484.4341	-0.0014	0.025			
41:	6	1	6	5	0	5	3484.5371	-0.0006	0.025			
42:	5	3	3	4	2	2	3535.9281	-0.0001	0.025			
43:	6	1	5	5	2	4	3686.0680	-0.0024	0.025			
44:	6	2	5	5	2	4	3691.1004	-0.0019	0.025			
45:	6	1	5	5	1	4	3704.1679	-0.0029	0.025			
46:	6	2	5	5	1	4	3709.2005	-0.0022	0.025			
47:	5	3	2	4	2	2	3765.7999	-0.0027	0.025			
48:	5	2	3	4	1	3	3768.1980	-0.0029	0.025			
49:	6	2	4	5	3	3	3785.1008	-0.0014	0.025			
50:	5	1	4	4	0	4	3844.8968	-0.0016	0.025			
51:	5	2	4	4	1	4	3860.7929	-0.0030	0.025			
52:	6	3	4	5	3	3	3861.1271	-0.0028	0.025			
53:	5	3	3	4	2	3	3883.0091	-0.0025	0.025			
54:	5	4	2	4	3	1	3910.3346	-0.0030	0.025			
55:	5	4	1	4	3	1	3942.1546	-0.0016	0.025			
56:	6	2	4	5	2	3	3954.2314	-0.0018	0.025			
57:	5	4	2	4	3	2	3989.5799	-0.0032	0.025			
58:	6	3	4	5	2	3	4030.2596	-0.0013	0.025			
59:	7	0	7	6	1	6	4047.1874	-0.0045	0.025	-0.0147	0.50	
60:	7	1	7	6	1	6	4047.1874	-0.0249	0.025	-0.0147	0.50	
61:	7	0	7	6	0	6	4047.3165	0.0224	0.025	0.0122	0.50	
62:	7	1	7	6	0	6	4047.3165	0.0020	0.025	0.0122	0.50	
63:	6	3	3	5	3	2	4092.7159	-0.0032	0.025			
64:	5	3	2	4	2	3	4112.8819	-0.0042	0.025			

65:	5	5	1	4	4	0	4163.7786	-0.0032	0.025		
66:	5	5	0	4	4	0	4164.8456	-0.0025	0.025		
67:	5	5	1	4	4	1	4167.8142	-0.0037	0.025		
68:	5	5	0	4	4	1	4168.8821	-0.0021	0.025		
69:	7	1	6	6	2	5	4256.6230	-0.0027	0.025		
70:	7	2	6	6	2	5	4257.8759	-0.0032	0.025		
71:	7	2	6	6	1	5	4262.9092	-0.0020	0.025		
72:	7	3	4	6	4	3	4372.9873	-0.0020	0.025		
73:	7	2	5	6	3	4	4426.3287	-0.0032	0.025		
74:	6	4	3	5	3	2	4453.7361	-0.0026	0.025		
75:	6	3	3	5	2	3	4491.7215	-0.0031	0.025		
76:	7	2	5	6	2	4	4502.3574	-0.0023	0.025		
77:	7	3	5	6	2	4	4529.1697	0.0003	0.025		
78:	6	2	4	5	1	4	4569.3116	-0.0041	0.025		
79:	6	4	2	5	3	2	4577.4714	-0.0040	0.025		
80:	7	4	4	6	4	3	4581.8891	-0.0038	0.025		
81:	8	0	8	7	1	7	4610.2748	0.0083	0.025	-0.0038	0.25
82:	8	1	8	7	1	7	4610.2748	0.0044	0.025	-0.0038	0.25
83:	8	0	8	7	0	7	4610.2748	-0.0120	0.025	-0.0038	0.25
84:	8	1	8	7	0	7	4610.2748	-0.0159	0.025	-0.0038	0.25
85:	7	5	3	6	5	2	4615.2599	-0.0047	0.025		
86:	6	1	5	5	0	5	4626.9476	0.0097	0.025		
87:	6	3	4	5	2	4	4627.2404	-0.0026	0.025		
88:	6	2	5	5	1	5	4631.4781	-0.0016	0.025		
89:	7	5	2	6	5	1	4658.0165	0.0098	0.025		
90:	6	4	3	5	3	3	4683.6089	-0.0043	0.025		
91:	7	3	4	6	3	3	4734.0063	-0.0026	0.025		
92:	7	4	3	6	4	2	4766.8946	-0.0032	0.025		
93:	6	5	2	5	4	1	4796.7219	-0.0045	0.025		
94:	8	1	7	7	2	6	4821.5434	-0.0033	0.025		
95:	8	2	7	7	2	6	4821.8344	-0.0026	0.025		
96:	8	1	7	7	1	6	4822.7972	-0.0030	0.025		
97:	8	2	7	7	1	6	4823.0883	-0.0022	0.025		
98:	6	5	2	5	4	2	4828.5401	-0.0049	0.025		
99:	6	5	1	5	4	2	4839.1548	-0.0041	0.025		
100:	8	4	4	7	5	3	4853.7125	-0.0033	0.025		
101:	7	4	4	6	3	3	4942.9094	-0.0030	0.025		
102:	6	6	0	5	5	0	5019.2639	-0.0022	0.025		
103:	6	6	1	5	5	1	5020.0661	-0.0027	0.025		
104:	6	6	0	5	5	1	5020.3302	-0.0021	0.025		
105:	8	2	6	7	3	5	5021.1136	-0.0051	0.025		
106:	8	3	6	7	3	5	5029.1307	-0.0028	0.025		
107:	8	3	6	7	2	5	5055.9393	-0.0039	0.025		
108:	6	3	3	5	2	4	5088.7014	-0.0052	0.025		
109:	8	3	5	7	4	4	5103.5952	-0.0030	0.025		
110:	8	4	5	7	4	4	5198.6964	-0.0034	0.025		
111:	7	4	3	6	3	3	5251.6495	-0.0047	0.025		
112:	9	5	4	8	6	3	5252.1732	0.0056	0.025		
113:	7	3	4	6	2	4	5271.4964	-0.0039	0.025		
114:	8	6	3	7	6	2	5276.7852	-0.0024	0.025		
115:	8	5	4	7	5	3	5278.0520	-0.0041	0.025		
116:	8	3	5	7	3	4	5312.4980	-0.0038	0.025		
117:	7	2	5	6	1	5	5367.5008	-0.0038	0.025		
118:	7	5	3	6	4	2	5378.8896	-0.0044	0.025		
119:	9	1	8	8	2	7	5384.9049	-0.0033	0.025		
120:	9	2	8	8	2	7	5384.9744	0.0023	0.025		
121:	9	1	8	8	1	7	5385.1827	-0.0159	0.025		
122:	9	2	8	8	1	7	5385.2613	-0.0011	0.025		
123:	7	3	5	6	2	5	5389.2782	-0.0041	0.025		
124:	8	5	3	7	5	2	5396.3142	-0.0031	0.025		
125:	7	1	6	6	0	6	5404.1575	-0.0025	0.025		
126:	7	4	4	6	3	4	5404.3714	-0.0047	0.025		
127:	7	2	6	6	1	6	5405.3073	-0.0040	0.025		
128:	8	4	5	7	3	4	5407.6001	-0.0032	0.025		
129:	7	5	2	6	4	2	5432.2455	-0.0044	0.025		
130:	8	4	4	7	4	3	5465.7078	-0.0041	0.025		
131:	6	4	3	5	1	4	5467.8211	-0.0055	0.025		
132:	7	5	3	6	4	3	5502.6255	-0.0053	0.025		
133:	7	5	2	6	4	3	5555.9826	-0.0040	0.025		
134:	9	2	7	8	3	6	5594.3653	-0.0038	0.025		

135:	9	2	7	8	2	6	5602.3798	-0.0042	0.025		
136:	9	3	7	8	2	6	5604.5355	-0.0029	0.025		
137:	7	6	2	6	5	1	5665.2754	-0.0054	0.025		
138:	7	6	1	6	5	1	5668.4287	-0.0050	0.025		
139:	7	6	2	6	5	2	5675.8900	-0.0047	0.025		
140:	9	4	5	8	5	4	5677.8208	-0.0034	0.025		
141:	7	6	1	6	5	2	5679.0431	-0.0045	0.025		
142:	7	4	3	6	3	4	5713.1117	-0.0061	0.025		
143:	10	0	10	9	1	9	5736.3250	-0.0018	0.025	-0.0023	0.25
144:	10	1	10	9	0	9	5736.3250	-0.0027	0.025	-0.0023	0.25
145:	10	0	10	9	0	9	5736.3250	-0.0026	0.025	-0.0023	0.25
146:	10	1	10	9	1	9	5736.3250	-0.0020	0.025	-0.0023	0.25
147:	9	3	6	8	4	5	5757.4735	-0.0036	0.025		
148:	9	4	6	8	4	5	5792.2963	-0.0036	0.025		
149:	9	3	6	8	3	5	5852.5729	-0.0058	0.025		
150:	7	7	1	6	6	0	5872.7486	-0.0044	0.025		
151:	7	7	0	6	6	0	5872.8084	-0.0069	0.025	-0.0069	0.50
152:	7	7	0	6	6	0	5872.8084	-0.0069	0.025	-0.0069	0.50
153:	7	7	1	6	6	1	5873.0091	-0.0075	0.025		
154:	7	7	0	6	6	1	5873.0760	-0.0029	0.025		
155:	9	4	6	8	3	5	5887.3981	-0.0033	0.025		
156:	8	5	4	7	4	3	5890.0486	-0.0037	0.025		
157:	9	5	5	8	5	4	5921.4181	-0.0035	0.025		
158:	9	7	3	8	7	2	5932.2269	-0.0049	0.025		
159:	9	7	2	8	7	1	5937.5861	-0.0048	0.025		
160:	10	1	9	9	2	8	5947.8956	-0.0147	0.025	-0.0215	0.50
161:	10	2	9	9	2	8	5947.8956	-0.0282	0.025	-0.0215	0.50
162:	10	1	9	9	1	8	5947.9897	0.0155	0.025	0.0088	0.50
163:	10	2	9	9	1	8	5947.9897	0.0020	0.025	0.0088	0.50
164:	9	6	4	8	6	3	5953.5293	0.0062	0.025		
165:	8	4	4	7	3	4	5983.3531	-0.0042	0.025		
166:	9	6	3	8	6	2	6012.1784	-0.0053	0.025		
167:	8	5	3	7	4	3	6061.6641	-0.0053	0.025		
168:	8	3	5	7	2	5	6081.6380	-0.0043	0.025		
169:	9	4	5	8	4	4	6102.1615	-0.0030	0.025		
170:	7	3	4	6	2	5	6131.6017	-0.0114	0.025		
171:	10	5	5	9	6	4	6138.9954	-0.0018	0.025		
172:	9	5	4	8	5	3	6139.9086	-0.0035	0.025		
173:	8	4	5	7	3	5	6149.9299	-0.0044	0.025		
174:	8	2	6	7	1	6	6153.7716	-0.0036	0.025		
175:	8	3	6	7	2	6	6160.5318	-0.0048	0.025		
176:	10	2	8	9	2	7	6162.0801	-0.0042	0.025		
177:	10	3	8	9	2	7	6162.6203	-0.0019	0.025		
178:	8	1	7	7	0	7	6179.6668	0.0005	0.025		
179:	8	2	7	7	1	7	6179.9298	-0.0063	0.025		
180:	8	5	4	7	4	4	6198.7887	-0.0054	0.025		
181:	8	6	3	7	5	2	6284.0568	-0.0050	0.025		
182:	11	0	11	10	1	10	6299.3366	-0.0041	0.025	-0.0042	0.25
183:	11	1	11	10	1	10	6299.3366	-0.0041	0.025	-0.0042	0.25
184:	11	0	11	10	0	10	6299.3366	-0.0042	0.025	-0.0042	0.25
185:	11	1	11	10	0	10	6299.3366	-0.0042	0.025	-0.0042	0.25
186:	8	6	2	7	5	2	6303.3772	-0.0054	0.025		
187:	8	6	3	7	5	3	6337.4122	-0.0054	0.025		
188:	7	4	4	6	1	5	6345.5454	-0.0033	0.025		
189:	8	6	2	7	5	3	6356.7334	-0.0050	0.025		
190:	10	3	7	9	4	6	6358.0235	-0.0038	0.025		
191:	10	4	7	9	4	6	6368.9766	-0.0039	0.025		
192:	8	5	3	7	4	4	6370.4062	-0.0049	0.025		
193:	7	5	3	6	2	4	6401.1334	-0.0083	0.025		
194:	11	1	10	10	2	9	6510.8532	0.0038	0.025	-0.0043	0.25
195:	11	2	10	10	2	9	6510.8532	0.0010	0.025	-0.0043	0.25
196:	11	1	10	10	1	9	6510.8532	-0.0096	0.025	-0.0043	0.25
197:	11	2	10	10	1	9	6510.8532	-0.0124	0.025	-0.0043	0.25
198:	8	7	2	7	6	1	6524.0135	-0.0063	0.025		
199:	8	7	1	7	6	1	6524.8835	-0.0044	0.025		
200:	8	7	2	7	6	2	6527.1667	-0.0059	0.025		
201:	8	7	1	7	6	2	6528.0373	-0.0033	0.025		
202:	10	5	6	9	5	5	6539.5813	-0.0036	0.025		
203:	10	8	2	9	8	1	6587.0903	-0.0094	0.025		
204:	10	7	4	9	7	3	6615.2324	-0.0026	0.025		

205:	10	6	5	9	6	4	6619.4130	-0.0015	0.025		
206:	10	7	3	9	7	2	6639.0082	-0.0050	0.025		
207:	10	4	6	9	4	5	6671.2970	-0.0039	0.025		
208:	11	2	9	10	3	8	6723.2430	-0.0054	0.025		
209:	11	2	9	10	2	8	6723.7809	-0.0053	0.025		
210:	11	3	9	10	2	8	6723.9086	-0.0048	0.025		
211:	8	4	4	7	3	5	6725.6866	-0.0016	0.025		
212:	8	8	1	7	7	1	6726.1487	0.0123	0.025	0.0052	0.50
213:	8	8	0	7	7	1	6726.1487	-0.0018	0.025	0.0052	0.50
214:	9	5	4	8	4	4	6735.8651	-0.0043	0.025		
215:	10	6	4	9	6	3	6764.2919	-0.0038	0.025		
216:	9	4	5	8	3	5	6773.0160	-0.0040	0.025		
217:	10	5	6	9	4	5	6783.1781	-0.0044	0.025		
218:	10	5	5	9	5	4	6840.3475	-0.0052	0.025		
219:	9	6	4	8	5	3	6841.2619	-0.0055	0.025		
220:	12	0	12	11	1	11	6862.3393	-0.0041	0.025	-0.0041	0.25
221:	12	1	12	11	1	11	6862.3393	-0.0041	0.025	-0.0041	0.25
222:	12	0	12	11	0	11	6862.3393	-0.0041	0.025	-0.0041	0.25
223:	12	1	12	11	0	11	6862.3393	-0.0041	0.025	-0.0041	0.25
224:	9	3	6	8	2	6	6886.2872	-0.0055	0.025		
225:	9	4	6	8	3	6	6913.0952	-0.0054	0.025		
226:	9	6	3	8	5	3	6919.2432	-0.0057	0.025		
227:	9	5	5	8	4	5	6921.5101	-0.0057	0.025		
228:	11	3	8	10	4	7	6933.2907	-0.0047	0.025		
229:	9	3	7	8	2	7	6935.2163	-0.0069	0.025		
230:	11	4	8	10	4	7	6936.4079	-0.0005	0.025		
231:	11	3	8	10	3	7	6944.2428	-0.0060	0.025		
232:	11	4	8	10	3	7	6947.3566	-0.0052	0.025		
233:	11	5	6	10	6	5	6990.3115	-0.0027	0.025		
234:	9	6	4	8	5	4	7012.8793	-0.0053	0.025		
235:	12	1	11	11	2	10	7073.7816	-0.0023	0.025	-0.0040	0.25
236:	12	2	11	11	2	10	7073.7816	-0.0028	0.025	-0.0040	0.25
237:	12	1	11	11	1	10	7073.7816	-0.0051	0.025	-0.0040	0.25
238:	12	2	11	11	1	10	7073.7816	-0.0056	0.025	-0.0040	0.25
239:	9	6	3	8	5	4	7090.8604	-0.0055	0.025		
240:	11	4	7	10	5	6	7091.6088	-0.0037	0.025		
241:	11	5	7	10	5	6	7133.7002	-0.0057	0.025		
242:	9	7	3	8	6	2	7163.2897	-0.0064	0.025		
243:	9	7	2	8	6	2	7169.5170	-0.0064	0.025		
244:	8	5	4	7	2	5	7176.8344	-0.0037	0.025		
245:	9	7	3	8	6	3	7182.6099	-0.0068	0.025		
246:	9	7	2	8	6	3	7188.8374	-0.0067	0.025		
247:	11	5	7	10	4	6	7245.5820	-0.0054	0.025		
248:	11	8	4	10	8	3	7269.8760	-0.0073	0.025		
249:	11	8	3	10	8	2	7278.3070	-0.0088	0.025		
250:	8	4	5	7	1	6	7282.5827	-0.0081	0.025		
251:	11	7	5	10	7	4	7295.9154	-0.0065	0.025		
252:	9	5	4	8	4	5	7311.6158	-0.0075	0.025		
253:	10	6	5	9	5	4	7320.7640	-0.0059	0.025		
254:	11	7	4	10	7	3	7371.4576	-0.0208	0.025		
255:	9	8	2	8	7	2	7379.8738	-0.0091	0.025		
256:	9	8	1	8	7	2	7380.1056	-0.0038	0.025		
257:	13	0	13	12	0	12	7425.3269	-0.0065	0.025	-0.0065	0.25
258:	13	0	13	12	1	12	7425.3269	-0.0065	0.025	-0.0065	0.25
259:	13	1	13	12	0	12	7425.3269	-0.0065	0.025	-0.0065	0.25
260:	13	1	13	12	1	12	7425.3269	-0.0065	0.025	-0.0065	0.25
261:	11	5	6	10	5	5	7470.7288	-0.0027	0.025		
262:	10	5	5	9	4	5	7474.0531	-0.0046	0.025		
263:	12	3	9	11	4	8	7499.2066	-0.0070	0.025		
264:	12	4	9	11	4	8	7500.0264	-0.0100	0.025		
265:	12	3	9	11	3	8	7502.3188	-0.0078	0.025		
266:	12	4	9	11	3	8	7503.1460	-0.0033	0.025		
267:	10	6	4	9	5	4	7543.6259	-0.0067	0.025		
268:	9	9	1	8	8	0	7579.2639	0.0027	0.025	-0.0059	0.25
269:	9	9	0	8	8	0	7579.2639	-0.0004	0.025	-0.0059	0.25
270:	9	9	1	8	8	1	7579.2639	-0.0114	0.025	-0.0059	0.25
271:	9	9	0	8	8	1	7579.2639	-0.0146	0.025	-0.0059	0.25
272:	10	4	6	9	3	6	7591.7374	-0.0048	0.025		
273:	13	1	12	12	2	11	7636.7140	-0.0055	0.025	-0.0059	0.25
274:	13	2	12	12	2	11	7636.7140	-0.0056	0.025	-0.0059	0.25

275:	13	1	12	12	1	11	7636.7140	-0.0061	0.025	-0.0059	0.25
276:	13	2	12	12	1	11	7636.7140	-0.0062	0.025	-0.0059	0.25
277:	10	5	6	9	4	6	7668.7939	-0.0071	0.025		
278:	10	3	7	9	2	7	7676.7544	-0.0043	0.025		
279:	10	4	7	9	3	7	7685.5514	-0.0062	0.025		
280:	10	2	8	9	1	8	7710.2447	-0.0001	0.025		
281:	12	5	8	11	5	7	7710.3708	-0.0057	0.025		
282:	10	3	8	9	2	8	7710.7110	-0.0079	0.025		
283:	10	6	5	9	5	5	7710.8701	-0.0073	0.025		
284:	10	1	9	9	0	9	7729.2511	0.0059	0.025	-0.0004	0.50
285:	10	2	9	9	1	9	7729.2511	-0.0067	0.025	-0.0004	0.50
286:	12	4	8	11	4	7	7738.7192	0.0027	0.025		
287:	11	6	6	10	5	5	7744.7282	-0.0055	0.025		
288:	12	5	8	11	4	7	7752.4651	-0.0047	0.025		
289:	12	5	7	11	6	6	7756.2934	-0.0011	0.025		
290:	10	7	4	9	6	3	7766.3427	-0.0047	0.025		
291:	10	7	3	9	6	3	7796.3463	-0.0065	0.025		
292:	10	7	4	9	6	4	7844.3226	-0.0062	0.025		
293:	13	2	11	12	3	10	7848.7963	0.0120	0.025	-0.0055	0.25
294:	13	3	11	12	3	10	7848.7963	0.0057	0.025	-0.0055	0.25
295:	13	2	11	12	2	10	7848.7963	-0.0167	0.025	-0.0055	0.25
296:	13	3	11	12	2	10	7848.7963	-0.0230	0.025	-0.0055	0.25
297:	10	7	3	9	6	4	7874.3284	-0.0059	0.025		
298:	10	6	4	9	5	5	7933.7358	-0.0043	0.025		
299:	12	7	6	11	7	5	7964.0394	0.0003	0.025		
300:	14	0	14	13	0	13	7988.3016	-0.0073	0.025	-0.0074	0.25
301:	14	1	14	13	1	13	7988.3016	-0.0073	0.025	-0.0074	0.25
302:	14	1	14	13	0	13	7988.3016	-0.0073	0.025	-0.0074	0.25
303:	14	0	14	13	1	13	7988.3016	-0.0073	0.025	-0.0074	0.25
304:	10	8	3	9	7	2	8026.9011	0.0053	0.025		
305:	10	8	2	9	7	2	8028.7548	0.0046	0.025		
306:	10	8	3	9	7	3	8033.1292	0.0061	0.025		
307:	10	8	2	9	7	3	8034.9842	0.0066	0.025		
308:	9	5	5	8	2	6	8050.3362	0.0046	0.025		
309:	13	3	10	12	4	9	8062.3204	0.0002	0.025		
310:	13	4	10	12	3	9	8063.3557	0.0071	0.025		
311:	9	6	4	8	3	5	8108.0802	-0.0002	0.025		
312:	12	6	7	11	5	6	8156.9324	0.0048	0.025		
313:	14	1	13	13	2	12	8199.6557	0.0039	0.025	0.0039	0.25
314:	14	2	13	13	1	12	8199.6557	0.0038	0.025	0.0039	0.25
315:	14	1	13	13	1	12	8199.6557	0.0038	0.025	0.0039	0.25
316:	14	2	13	13	2	12	8199.6557	0.0039	0.025	0.0039	0.25
317:	11	6	5	10	5	5	8218.9525	0.0065	0.025		
318:	10	9	2	9	8	1	8232.7809	0.0122	0.025	-0.0161	0.50
319:	10	9	1	9	8	1	8232.7809	-0.0445	0.025	-0.0161	0.50
320:	10	9	2	9	8	2	8233.0488	0.0537	0.025	0.0253	0.50
321:	10	9	1	9	8	2	8233.0488	-0.0030	0.025	0.0253	0.50
322:	13	4	9	12	5	8	8273.3549	0.0014	0.025		
323:	11	5	6	10	4	6	8273.4980	0.0097	0.025		
324:	13	5	9	12	5	8	8277.4400	0.0061	0.025		
325:	13	4	9	12	4	8	8287.1129	0.0061	0.025		
326:	13	5	9	12	4	8	8291.1953	0.0080	0.025		
327:	11	7	5	10	6	4	8297.9777	0.0040	0.025		
328:	13	6	7	12	7	6	8309.0489	0.0122	0.025		
329:	10	5	5	9	4	6	8359.6838	0.0075	0.025		
330:	11	4	7	10	3	7	8402.3933	0.0070	0.025		
331:	11	7	4	10	6	4	8403.5346	-0.0009	0.025		
332:	14	2	12	13	3	11	8411.5557	0.0116	0.025	0.0078	0.25
333:	14	3	12	13	3	11	8411.5557	0.0102	0.025	0.0078	0.25
334:	14	2	12	13	2	11	8411.5557	0.0053	0.025	0.0078	0.25
335:	14	3	12	13	2	11	8411.5557	0.0039	0.025	0.0078	0.25
336:	13	5	8	12	6	7	8428.2521	0.0044	0.025		
337:	10	10	1	9	9	0	8432.3990	0.0086	0.025	0.0067	0.25
338:	10	10	0	9	9	1	8432.3990	0.0047	0.025	0.0067	0.25
339:	10	10	0	9	9	0	8432.3990	0.0079	0.025	0.0067	0.25
340:	10	10	1	9	9	1	8432.3990	0.0054	0.025	0.0067	0.25
341:	11	6	6	10	5	6	8435.6148	0.0058	0.025		
342:	11	3	8	10	2	8	8458.9290	0.0057	0.025		
343:	13	6	8	12	6	7	8476.9001	0.0200	0.025		
344:	11	1	10	10	0	10	8503.7790	-0.0012	0.025	-0.0026	0.50

345:	11	2	10	10	1	10	8503.7790	-0.0038	0.025	-0.0026	0.50
346:	11	7	5	10	6	5	8520.8389	0.0026	0.025		
347:	13	6	8	12	5	7	8603.5171	0.0064	0.025		
348:	11	7	4	10	6	5	8626.4041	0.0058	0.025		
349:	11	8	4	10	7	3	8657.7714	0.0055	0.025		
350:	11	8	3	10	7	3	8668.0542	0.0014	0.025		
351:	11	8	3	10	7	4	8698.0632	0.0049	0.025		
352:	16	10	7	15	11	4	8711.2059	0.0175	0.025		
353:	12	7	6	11	6	5	8746.3512	0.0045	0.025		
354:	15	1	14	14	2	13	8762.5825	0.0064	0.025	0.0065	0.25
355:	15	2	14	14	2	13	8762.5825	0.0064	0.025	0.0065	0.25
356:	15	1	14	14	1	13	8762.5825	0.0064	0.025	0.0065	0.25
357:	15	2	14	14	1	13	8762.5825	0.0064	0.025	0.0065	0.25
358:	14	4	10	13	5	9	8839.3841	0.0043	0.025		
359:	14	5	10	13	4	9	8844.5983	0.0099	0.025		
360:	11	9	3	10	8	2	8883.8838	0.0043	0.025		
361:	11	9	2	10	8	2	8884.4049	0.0042	0.025		
362:	11	9	3	10	8	3	8885.7389	0.0050	0.025		
363:	11	9	2	10	8	3	8886.2611	0.0060	0.025		
364:	11	6	5	10	5	6	8909.8286	0.0074	0.025		
365:	16	9	8	15	10	5	8934.8240	0.0263	0.025		
366:	12	6	6	11	5	6	8964.2407	0.0056	0.025		
367:	15	2	13	14	3	12	8974.3371	0.0047	0.025	0.0040	0.25
368:	15	3	13	14	3	12	8974.3371	0.0045	0.025	0.0040	0.25
369:	15	2	13	14	2	12	8974.3371	0.0034	0.025	0.0040	0.25
370:	15	3	13	14	2	12	8974.3371	0.0031	0.025	0.0040	0.25
371:	10	5	6	9	2	7	8987.5377	0.0052	0.025		
372:	12	7	5	11	6	5	9023.8066	0.0060	0.025		
373:	14	5	9	13	6	8	9036.7075	0.0088	0.025		
374:	14	6	8	13	7	7	9088.5933	0.0096	0.025		
375:	12	5	7	11	4	7	9100.2970	0.0060	0.025		
376:	14	6	9	13	5	8	9101.7075	0.0067	0.025		
377:	16	0	16	15	0	15	9114.2177	0.0064	0.025	0.0064	0.25
378:	16	0	16	15	1	15	9114.2177	0.0064	0.025	0.0064	0.25
379:	16	1	16	15	0	15	9114.2177	0.0064	0.025	0.0064	0.25
380:	16	1	16	15	1	15	9114.2177	0.0064	0.025	0.0064	0.25
381:	10	7	4	9	4	5	9179.3873	-0.0019	0.025		
382:	12	6	7	11	5	7	9184.8325	0.0041	0.025		
383:	12	4	8	11	3	8	9196.8589	0.0048	0.025		
384:	12	7	6	11	6	6	9220.5617	0.0028	0.025		
385:	10	4	7	9	1	8	9235.8733	0.0007	0.025		
386:	12	3	9	11	2	9	9237.4682	0.0046	0.025		
387:	12	4	9	11	3	9	9238.1565	-0.0027	0.025		
388:	12	8	5	11	7	4	9243.8652	0.0016	0.025		
389:	12	1	11	11	0	11	9278.2283	0.0020	0.025	0.0018	0.50
390:	12	2	11	11	1	11	9278.2283	0.0015	0.025	0.0018	0.50
391:	11	11	1	10	10	0	9285.4851	0.0051	0.025	0.0047	0.25
392:	11	11	0	10	10	1	9285.4851	0.0042	0.025	0.0047	0.25
393:	11	11	1	10	10	1	9285.4851	0.0044	0.025	0.0047	0.25
394:	11	11	0	10	10	0	9285.4851	0.0049	0.025	0.0047	0.25
395:	12	8	4	11	7	4	9286.4807	0.0011	0.025		
396:	16	1	15	15	1	14	9325.4936	0.0048	0.025	0.0049	0.25
397:	16	1	15	15	2	14	9325.4936	0.0048	0.025	0.0049	0.25
398:	16	2	15	15	1	14	9325.4936	0.0048	0.025	0.0049	0.25
399:	16	2	15	15	2	14	9325.4936	0.0048	0.025	0.0049	0.25
400:	12	8	5	11	7	5	9349.4387	0.0131	0.025		
401:	16	9	7	15	10	6	9352.8517	0.0236	0.025		
402:	14	6	8	13	6	7	9389.2782	0.0132	0.025		
403:	12	8	4	11	7	5	9392.0471	0.0056	0.025		
404:	15	4	11	14	5	10	9402.1257	0.0017	0.025		
405:	15	5	11	14	4	10	9403.5499	0.0026	0.025		
406:	11	5	6	10	4	7	9461.4359	0.0087	0.025		
407:	12	7	5	11	6	6	9498.0188	0.0061	0.025		
408:	12	9	4	11	8	3	9527.4150	0.0028	0.025		
409:	14	7	8	13	6	7	9528.8366	0.0041	0.025		
410:	12	9	3	11	8	3	9530.6726	0.0055	0.025		
411:	16	2	14	15	3	13	9537.1398	0.0018	0.025	0.0016	0.25
412:	16	3	14	15	3	13	9537.1398	0.0017	0.025	0.0016	0.25
413:	16	2	14	15	2	13	9537.1398	0.0015	0.025	0.0016	0.25
414:	16	3	14	15	2	13	9537.1398	0.0014	0.025	0.0016	0.25

415:	17	9	9	16	10	6	9537.7039	0.0321	0.025	0.0185	0.50
416:	12	9	4	11	8	4	9537.7039	0.0047	0.025	0.0185	0.50
417:	12	9	3	11	8	4	9540.9581	0.0041	0.025		
418:	15	5	10	14	6	9	9614.4422	0.0066	0.025		
419:	15	6	10	14	5	9	9635.8384	0.0064	0.025		
420:	17	0	17	16	0	16	9677.1388	0.0033	0.025	0.0034	0.25
421:	17	0	17	16	1	16	9677.1388	0.0033	0.025	0.0034	0.25
422:	17	1	17	16	0	16	9677.1388	0.0033	0.025	0.0034	0.25
423:	17	1	17	16	1	16	9677.1388	0.0033	0.025	0.0034	0.25
424:	13	7	6	12	6	6	9701.2174	0.0050	0.025		
425:	12	10	3	11	9	2	9738.4504	0.0016	0.025		
426:	12	10	2	11	9	2	9738.6033	0.0143	0.025		
427:	12	10	3	11	9	3	9738.9604	-0.0095	0.025		
428:	12	10	2	11	9	3	9739.1148	0.0046	0.025		
429:	13	8	6	12	7	5	9749.4108	0.0110	0.025		
430:	16	3	13	15	4	12	9749.7106	0.0105	0.025	0.0036	0.25
431:	16	4	13	15	4	12	9749.7106	0.0080	0.025	0.0036	0.25
432:	16	3	13	15	3	12	9749.7106	-0.0008	0.025	0.0036	0.25
433:	16	4	13	15	3	12	9749.7106	-0.0033	0.025	0.0036	0.25
434:	13	6	7	12	5	7	9773.3139	0.0130	0.025		
435:	17	1	16	16	1	15	9888.3936	0.0067	0.025	0.0067	0.25
436:	17	1	16	16	2	15	9888.3936	0.0067	0.025	0.0067	0.25
437:	17	2	16	16	1	15	9888.3936	0.0067	0.025	0.0067	0.25
438:	17	2	16	16	2	15	9888.3936	0.0067	0.025	0.0067	0.25
439:	13	7	7	12	6	7	9947.3340	-0.0174	0.025		
440:	13	6	8	12	5	8	9951.2953	-0.0365	0.025		
441:	13	8	6	12	7	6	10026.8533	-0.0003	0.025		
442:	13	9	5	12	8	4	10148.7579	0.0077	0.025		
443:	13	8	5	12	7	6	10162.9031	0.0079	0.025		
444:	13	9	4	12	8	4	10164.1112	0.0127	0.025		
445:	14	8	7	13	7	6	10167.1263	0.0039	0.025		
446:	16	5	11	15	6	10	10180.3620	0.0026	0.025		
447:	18	0	18	17	0	17	10240.0671	0.0272	0.025	0.0272	0.25
448:	18	0	18	17	1	17	10240.0671	0.0272	0.025	0.0272	0.25
449:	18	1	18	17	0	17	10240.0671	0.0272	0.025	0.0272	0.25
450:	18	1	18	17	1	17	10240.0671	0.0272	0.025	0.0272	0.25
451:	17	3	14	16	4	13	10312.2723	0.0076	0.025	0.0061	0.25
452:	17	4	14	16	4	13	10312.2723	0.0071	0.025	0.0061	0.25
453:	17	3	14	16	3	13	10312.2723	0.0051	0.025	0.0061	0.25
454:	17	4	14	16	3	13	10312.2723	0.0045	0.025	0.0061	0.25
455:	13	10	4	12	9	3	10387.1070	0.0067	0.025		
456:	13	10	3	12	9	3	10388.0687	-0.0019	0.025		
457:	13	10	4	12	9	4	10390.3632	0.0080	0.025		
458:	13	10	3	12	9	4	10391.3365	0.0110	0.025		
459:	18	1	17	17	1	16	10451.2674	-0.0007	0.025	-0.0097	0.20
460:	18	1	17	17	2	16	10451.2674	-0.0007	0.025	-0.0097	0.20
461:	18	2	17	17	1	16	10451.2674	-0.0007	0.025	-0.0097	0.20
462:	18	2	17	17	2	16	10451.2674	-0.0007	0.025	-0.0097	0.20
463:	16	7	10	15	6	9	10451.2674	-0.0457	0.025	-0.0097	0.20
464:	14	8	6	13	7	6	10502.5017	0.0085	0.025		
465:	13	7	6	12	6	7	10508.5262	0.0063	0.025		
466:	18	2	16	17	2	15	10662.7676	0.0062	0.025	0.0063	0.25
467:	18	2	16	17	3	15	10662.7676	0.0063	0.025	0.0063	0.25
468:	18	3	16	17	2	15	10662.7676	0.0062	0.025	0.0063	0.25
469:	18	3	16	17	3	15	10662.7676	0.0063	0.025	0.0063	0.25
470:	12	6	7	11	3	8	10685.0735	0.0143	0.025		
471:	14	7	8	13	6	8	10698.6059	-0.0167	0.025		
472:	14	5	9	13	4	9	10714.6869	0.0098	0.025		
473:	14	9	6	13	8	5	10716.8434	0.0047	0.025		
474:	14	6	9	13	5	9	10726.9744	0.0081	0.025		
475:	14	8	7	13	7	7	10728.3003	0.0095	0.025		
476:	17	6	12	16	5	11	10744.4335	-0.0148	0.025		
477:	14	4	10	13	3	10	10761.9687	0.0170	0.025		
478:	14	5	10	13	4	10	10762.8799	0.0059	0.025		
479:	14	9	5	13	8	5	10773.9857	0.0005	0.025		
480:	13	12	2	12	11	1	10792.4053	0.0097	0.025	0.0077	0.25
481:	13	12	1	12	11	1	10792.4053	0.0089	0.025	0.0077	0.25
482:	13	12	2	12	11	2	10792.4053	0.0064	0.025	0.0077	0.25
483:	13	12	1	12	11	2	10792.4053	0.0057	0.025	0.0077	0.25
484:	19	0	19	18	0	18	10802.9286	0.0052	0.025	0.0052	0.25

485:	19	0	19	18	1	18	10802.9286	0.0052	0.025	0.0052	0.25
486:	19	1	19	18	0	18	10802.9286	0.0052	0.025	0.0052	0.25
487:	19	1	19	18	1	18	10802.9286	0.0052	0.025	0.0052	0.25
488:	14	2	12	13	1	12	10811.2336	0.0065	0.025	0.0059	0.50
489:	14	3	12	13	2	12	10811.2336	0.0053	0.025	0.0059	0.50
490:	14	9	6	13	8	6	10852.8872	0.0070	0.025		
491:	18	3	15	17	4	14	10874.8879	0.0078	0.025	0.0075	0.25
492:	18	4	15	17	4	14	10874.8879	0.0077	0.025	0.0075	0.25
493:	18	3	15	17	3	14	10874.8879	0.0073	0.025	0.0075	0.25
494:	18	4	15	17	3	14	10874.8879	0.0071	0.025	0.0075	0.25
495:	14	9	5	13	8	6	10910.0253	-0.0013	0.025		
496:	17	6	11	16	6	10	10975.1897	-0.0145	0.025		
497:	13	13	0	12	12	0	10991.5603	0.0133	0.025	0.0134	0.25
498:	13	13	0	12	12	1	10991.5603	0.0133	0.025	0.0134	0.25
499:	13	13	1	12	12	0	10991.5603	0.0133	0.025	0.0134	0.25
500:	13	13	1	12	12	1	10991.5603	0.0133	0.025	0.0134	0.25
501:	19	1	18	18	1	17	11014.1400	0.0096	0.025	0.0097	0.25
502:	19	1	18	18	2	17	11014.1400	0.0096	0.025	0.0097	0.25
503:	19	2	18	18	1	17	11014.1400	0.0096	0.025	0.0097	0.25
504:	19	2	18	18	2	17	11014.1400	0.0096	0.025	0.0097	0.25
505:	14	10	4	13	9	5	11045.9652	0.0083	0.025		
506:	15	8	7	14	7	7	11182.9091	0.0067	0.025		
507:	15	9	7	14	8	6	11195.8291	-0.0104	0.025		
508:	14	11	4	13	10	3	11242.8940	0.0108	0.025		
509:	14	11	3	13	10	3	11243.1759	0.0165	0.025		
510:	14	11	4	13	10	4	11243.8532	-0.0004	0.025		
511:	14	11	3	13	10	4	11244.1332	0.0035	0.025		
512:	15	7	8	14	6	8	11272.6910	0.0022	0.025		
513:	20	0	20	19	0	19	11365.7912	0.0065	0.025	0.0066	0.25
514:	20	0	20	19	1	19	11365.7912	0.0065	0.025	0.0066	0.25
515:	20	1	20	19	0	19	11365.7912	0.0065	0.025	0.0066	0.25
516:	20	1	20	19	1	19	11365.7912	0.0065	0.025	0.0066	0.25
517:	14	12	3	13	11	2	11445.5516	0.0316	0.025	0.0089	0.25
518:	14	12	2	13	11	2	11445.5516	0.0224	0.025	0.0089	0.25
519:	14	12	3	13	11	3	11445.5516	-0.0047	0.025	0.0089	0.25
520:	14	12	2	13	11	3	11445.5516	-0.0138	0.025	0.0089	0.25
521:	15	8	8	14	7	8	11457.2021	0.0104	0.025		
522:	17	10	7	16	10	6	11471.5080	-0.0002	0.025		
523:	15	6	10	14	5	10	11505.9246	0.0038	0.025		
524:	18	6	12	17	7	11	11522.0852	0.0187	0.025		
525:	20	1	19	19	1	18	11576.9737	0.0017	0.025	0.0017	0.25
526:	20	1	19	19	2	18	11576.9737	0.0017	0.025	0.0017	0.25
527:	20	2	19	19	1	18	11576.9737	0.0017	0.025	0.0017	0.25
528:	20	2	19	19	2	18	11576.9737	0.0017	0.025	0.0017	0.25
529:	15	10	6	14	9	5	11636.3440	0.0156	0.025		
530:	14	13	2	13	12	1	11645.4468	0.0132	0.025	0.0127	0.25
531:	14	13	1	13	12	1	11645.4468	0.0130	0.025	0.0127	0.25
532:	14	13	2	13	12	2	11645.4468	0.0124	0.025	0.0127	0.25
533:	14	13	1	13	12	2	11645.4468	0.0122	0.025	0.0127	0.25
534:	19	4	15	18	5	14	11650.5544	0.0038	0.025	0.0013	0.25
535:	19	5	15	18	5	14	11650.5544	0.0029	0.025	0.0013	0.25
536:	19	4	15	18	4	14	11650.5544	-0.0002	0.025	0.0013	0.25
537:	19	5	15	18	4	14	11650.5544	-0.0012	0.025	0.0013	0.25
538:	15	10	6	14	9	6	11693.4792	0.0043	0.025		
539:	15	9	6	14	8	7	11700.6269	0.0169	0.025		
540:	15	10	5	14	9	6	11714.9293	0.0143	0.025		
541:	18	7	11	17	8	10	11720.5122	-0.0075	0.025		
542:	19	9	10	18	10	8	11832.5134	-0.0368	0.025		
543:	14	14	0	13	13	0	11844.5314	0.0104	0.025	0.0104	0.25
544:	14	14	0	13	13	1	11844.5314	0.0104	0.025	0.0104	0.25
545:	14	14	1	13	13	0	11844.5314	0.0104	0.025	0.0104	0.25
546:	14	14	1	13	13	1	11844.5314	0.0104	0.025	0.0104	0.25
547:	15	11	5	14	10	4	11888.5891	0.0144	0.025		
548:	15	11	4	14	10	5	11895.2833	0.0126	0.025		
549:	21	0	21	20	0	20	11928.6304	0.0077	0.025	0.0078	0.25
550:	21	0	21	20	1	20	11928.6304	0.0077	0.025	0.0078	0.25
551:	21	1	21	20	0	20	11928.6304	0.0077	0.025	0.0078	0.25
552:	21	1	21	20	1	20	11928.6304	0.0077	0.025	0.0078	0.25
553:	21	1	20	20	1	19	12139.7949	0.0036	0.025	0.0036	0.25
554:	21	1	20	20	2	19	12139.7949	0.0036	0.025	0.0036	0.25

555:	21	2	20	20	1	19	12139.7949	0.0036	0.025	0.0036	0.25
556:	21	2	20	20	2	19	12139.7949	0.0036	0.025	0.0036	0.25
557:	20	4	16	19	5	15	12212.9167	0.0046	0.025	0.0040	0.25
558:	20	5	16	19	5	15	12212.9167	0.0044	0.025	0.0040	0.25
559:	20	4	16	19	4	15	12212.9167	0.0036	0.025	0.0040	0.25
560:	20	5	16	19	4	15	12212.9167	0.0034	0.025	0.0040	0.25
561:	15	13	3	14	12	2	12298.7285	0.0137	0.025	0.0081	0.25
562:	15	13	2	14	12	2	12298.7285	0.0115	0.025	0.0081	0.25
563:	15	13	3	14	12	3	12298.7285	0.0046	0.025	0.0081	0.25
564:	15	13	2	14	12	3	12298.7285	0.0023	0.025	0.0081	0.25
565:	22	0	22	21	0	21	12491.4369	0.0008	0.025	0.0008	0.25
566:	22	0	22	21	1	21	12491.4369	0.0008	0.025	0.0008	0.25
567:	22	1	22	21	0	21	12491.4369	0.0008	0.025	0.0008	0.25
568:	22	1	22	21	1	21	12491.4369	0.0008	0.025	0.0008	0.25
569:	15	14	2	14	13	1	12498.4233	0.0065	0.025	0.0065	0.25
570:	15	14	1	14	13	1	12498.4233	0.0065	0.025	0.0065	0.25
571:	15	14	1	14	13	2	12498.4233	0.0063	0.025	0.0065	0.25
572:	15	14	2	14	13	2	12498.4233	0.0064	0.025	0.0065	0.25
573:	15	15	0	14	14	0	12697.4643	0.0119	0.025	0.0120	0.25
574:	15	15	0	14	14	1	12697.4643	0.0119	0.025	0.0120	0.25
575:	15	15	1	14	14	0	12697.4643	0.0119	0.025	0.0120	0.25
576:	15	15	1	14	14	1	12697.4643	0.0119	0.025	0.0120	0.25
577:	22	1	21	21	1	20	12702.5822	-0.0044	0.025	-0.0044	0.25
578:	22	1	21	21	2	20	12702.5822	-0.0044	0.025	-0.0044	0.25
579:	22	2	21	21	1	20	12702.5822	-0.0044	0.025	-0.0044	0.25
580:	22	2	21	21	2	20	12702.5822	-0.0044	0.025	-0.0044	0.25
581:	16	12	5	15	11	4	12745.9574	-0.0023	0.025		
582:	16	12	4	15	11	4	12746.4386	0.0028	0.025		
583:	16	12	5	15	11	5	12747.5739	0.0185	0.025		
584:	16	12	4	15	11	5	12748.0361	0.0046	0.025		
585:	21	5	16	20	6	15	12989.2027	0.0094	0.025	0.0056	0.25
586:	21	6	16	20	6	15	12989.2027	0.0079	0.025	0.0056	0.25
587:	21	5	16	20	5	15	12989.2027	0.0032	0.025	0.0056	0.25
588:	21	6	16	20	5	15	12989.2027	0.0017	0.025	0.0056	0.25
589:	23	0	23	22	0	22	13054.2249	0.0011	0.025	0.0011	0.25
590:	23	0	23	22	1	22	13054.2249	0.0011	0.025	0.0011	0.25
591:	23	1	23	22	0	22	13054.2249	0.0011	0.025	0.0011	0.25
592:	23	1	23	22	1	22	13054.2249	0.0011	0.025	0.0011	0.25
593:	15	8	8	14	5	9	13119.0981	-0.0175	0.025		
594:	17	11	7	16	10	6	13120.5860	0.0147	0.025		
595:	22	3	19	21	3	18	13125.5209	-0.0031	0.025	-0.0032	0.25
596:	22	3	19	21	4	18	13125.5209	-0.0031	0.025	-0.0032	0.25
597:	22	4	19	21	3	18	13125.5209	-0.0031	0.025	-0.0032	0.25
598:	22	4	19	21	4	18	13125.5209	-0.0031	0.025	-0.0032	0.25
599:	16	14	3	15	13	2	13151.8052	0.0059	0.025	0.0046	0.25
600:	16	14	2	15	13	2	13151.8052	0.0054	0.025	0.0046	0.25
601:	16	14	3	15	13	3	13151.8052	0.0037	0.025	0.0046	0.25
602:	16	14	2	15	13	3	13151.8052	0.0031	0.025	0.0046	0.25
603:	23	1	22	22	1	21	13265.3551	-0.0017	0.025	-0.0018	0.25
604:	23	1	22	22	2	21	13265.3551	-0.0017	0.025	-0.0018	0.25
605:	23	2	22	22	1	21	13265.3551	-0.0017	0.025	-0.0018	0.25
606:	23	2	22	22	2	21	13265.3551	-0.0017	0.025	-0.0018	0.25
607:	16	15	1	15	14	1	13351.3542	0.0076	0.025	0.0076	0.25
608:	16	15	1	15	14	2	13351.3542	0.0075	0.025	0.0076	0.25
609:	16	15	2	15	14	1	13351.3542	0.0076	0.025	0.0076	0.25
610:	16	15	2	15	14	2	13351.3542	0.0075	0.025	0.0076	0.25
611:	17	12	5	16	11	5	13390.6853	0.0038	0.025		
612:	17	12	6	16	11	6	13395.6255	-0.0596	0.025		
613:	17	12	5	16	11	6	13398.1039	0.0005	0.025		
614:	23	2	21	22	2	20	13476.6199	-0.0011	0.025	-0.0011	0.25
615:	23	2	21	22	3	20	13476.6199	-0.0011	0.025	-0.0011	0.25
616:	23	3	21	22	2	20	13476.6199	-0.0011	0.025	-0.0011	0.25
617:	23	3	21	22	3	20	13476.6199	-0.0011	0.025	-0.0011	0.25
618:	16	16	0	15	15	0	13550.3484	0.0104	0.025	0.0104	0.25
619:	16	16	0	15	15	1	13550.3484	0.0104	0.025	0.0104	0.25
620:	16	16	1	15	15	0	13550.3484	0.0104	0.025	0.0104	0.25
621:	16	16	1	15	15	1	13550.3484	0.0104	0.025	0.0104	0.25
622:	22	5	17	21	6	16	13551.2428	0.0012	0.025	0.0003	0.25
623:	22	6	17	21	6	16	13551.2428	0.0009	0.025	0.0003	0.25
624:	22	5	17	21	5	16	13551.2428	-0.0002	0.025	0.0003	0.25

625:	22	6	17	21	5	16	13551.2428	-0.0005	0.025	0.0003	0.25
626:	24	0	24	23	0	23	13616.9877	0.0031	0.025	0.0031	0.25
627:	24	0	24	23	1	23	13616.9877	0.0031	0.025	0.0031	0.25
628:	24	1	24	23	0	23	13616.9877	0.0031	0.025	0.0031	0.25
629:	24	1	24	23	1	23	13616.9877	0.0031	0.025	0.0031	0.25
630:	20	10	11	19	9	10	13633.9119	-0.0076	0.025		
631:	23	3	20	22	3	19	13688.1752	-0.0057	0.025	-0.0057	0.25
632:	23	3	20	22	4	19	13688.1752	-0.0057	0.025	-0.0057	0.25
633:	23	4	20	22	3	19	13688.1752	-0.0057	0.025	-0.0057	0.25
634:	23	4	20	22	4	19	13688.1752	-0.0057	0.025	-0.0057	0.25
635:	24	1	23	23	1	22	13828.1009	0.0003	0.025	0.0004	0.25
636:	24	1	23	23	2	22	13828.1009	0.0003	0.025	0.0004	0.25
637:	24	2	23	23	1	22	13828.1009	0.0003	0.025	0.0004	0.25
638:	24	2	23	23	2	22	13828.1009	0.0003	0.025	0.0004	0.25
639:	23	4	19	22	4	18	13900.2979	0.0002	0.025	0.0002	0.25
640:	23	4	19	22	5	18	13900.2979	0.0002	0.025	0.0002	0.25
641:	23	5	19	22	4	18	13900.2979	0.0002	0.025	0.0002	0.25
642:	23	5	19	22	5	18	13900.2979	0.0002	0.025	0.0002	0.25
643:	17	15	3	16	14	2	14004.7962	-0.0001	0.025	-0.0005	0.25
644:	17	15	2	16	14	2	14004.7962	-0.0002	0.025	-0.0005	0.25
645:	17	15	3	16	14	3	14004.7962	-0.0006	0.025	-0.0005	0.25
646:	17	15	2	16	14	3	14004.7962	-0.0008	0.025	-0.0005	0.25
647:	24	2	22	23	2	21	14039.3241	-0.0077	0.025	-0.0077	0.25
648:	24	2	22	23	3	21	14039.3241	-0.0077	0.025	-0.0077	0.25
649:	24	3	22	23	2	21	14039.3241	-0.0077	0.025	-0.0077	0.25
650:	24	3	22	23	3	21	14039.3241	-0.0077	0.025	-0.0077	0.25
651:	23	5	18	22	6	17	14113.4001	0.0053	0.025	0.0052	0.25
652:	23	6	18	22	6	17	14113.4001	0.0053	0.025	0.0052	0.25
653:	23	5	18	22	5	17	14113.4001	0.0050	0.025	0.0052	0.25
654:	23	6	18	22	5	17	14113.4001	0.0049	0.025	0.0052	0.25
655:	17	16	1	16	15	1	14204.2213	-0.0014	0.025	-0.0015	0.25
656:	17	16	1	16	15	2	14204.2213	-0.0014	0.025	-0.0015	0.25
657:	17	16	2	16	15	1	14204.2213	-0.0014	0.025	-0.0015	0.25
658:	17	16	2	16	15	2	14204.2213	-0.0014	0.025	-0.0015	0.25
659:	25	1	24	24	1	23	14390.8153	-0.0009	0.025	-0.0009	0.25
660:	25	1	24	24	2	23	14390.8153	-0.0009	0.025	-0.0009	0.25
661:	25	2	24	24	1	23	14390.8153	-0.0009	0.025	-0.0009	0.25
662:	25	2	24	24	2	23	14390.8153	-0.0009	0.025	-0.0009	0.25
663:	17	17	0	16	16	0	14403.1790	0.0038	0.025	0.0039	0.25
664:	17	17	0	16	16	1	14403.1790	0.0038	0.025	0.0039	0.25
665:	17	17	1	16	16	0	14403.1790	0.0038	0.025	0.0039	0.25
666:	17	17	1	16	16	1	14403.1790	0.0038	0.025	0.0039	0.25
667:	17	8	9	16	7	10	14434.6339	-0.0226	0.025		
668:	24	4	20	23	4	19	14462.7970	-0.0043	0.025	-0.0044	0.25
669:	24	4	20	23	5	19	14462.7970	-0.0043	0.025	-0.0044	0.25
670:	24	5	20	23	4	19	14462.7970	-0.0043	0.025	-0.0044	0.25
671:	24	5	20	23	5	19	14462.7970	-0.0043	0.025	-0.0044	0.25
672:	19	10	10	18	9	10	14472.3032	0.0010	0.025		
673:	25	2	23	24	2	22	14602.0146	-0.0024	0.025	-0.0025	0.25
674:	25	2	23	24	3	22	14602.0146	-0.0024	0.025	-0.0025	0.25
675:	25	3	23	24	2	22	14602.0146	-0.0024	0.025	-0.0025	0.25
676:	25	3	23	24	3	22	14602.0146	-0.0024	0.025	-0.0025	0.25
677:	18	16	3	17	15	2	14857.6978	-0.0186	0.025	-0.0187	0.25
678:	18	16	2	17	15	2	14857.6978	-0.0186	0.025	-0.0187	0.25
679:	18	16	2	17	15	3	14857.6978	-0.0187	0.025	-0.0187	0.25
680:	18	16	3	17	15	3	14857.6978	-0.0187	0.025	-0.0187	0.25
681:	26	1	25	25	1	24	14953.4934	-0.0093	0.025	-0.0093	0.25
682:	26	1	25	25	2	24	14953.4934	-0.0093	0.025	-0.0093	0.25
683:	26	2	25	25	1	24	14953.4934	-0.0093	0.025	-0.0093	0.25
684:	26	2	25	25	2	24	14953.4934	-0.0093	0.025	-0.0093	0.25
685:	18	17	1	17	16	1	15057.0467	0.0025	0.025	0.0026	0.25
686:	18	17	1	17	16	2	15057.0467	0.0025	0.025	0.0026	0.25
687:	18	17	2	17	16	1	15057.0467	0.0025	0.025	0.0026	0.25
688:	18	17	2	17	16	2	15057.0467	0.0025	0.025	0.0026	0.25
689:	20	9	11	19	8	11	15124.9872	-0.0338	0.025		
690:	19	16	4	18	15	3	15510.5233	-0.0143	0.025	-0.0151	0.25
691:	19	16	3	18	15	3	15510.5233	-0.0146	0.025	-0.0151	0.25
692:	19	16	4	18	15	4	15510.5233	-0.0156	0.025	-0.0151	0.25
693:	19	16	3	18	15	4	15510.5233	-0.0159	0.025	-0.0151	0.25
694:	27	1	26	26	1	25	15516.1526	-0.0061	0.025	-0.0062	0.25

```
 695: 27  1 26   26  2 25                  15516.1526  -0.0061  0.025  -0.0062 0.25
 696: 27  2 26   26  1 25                  15516.1526  -0.0061  0.025  -0.0062 0.25
 697: 27  2 26   26  2 25                  15516.1526  -0.0061  0.025  -0.0062 0.25
 698: 26  4 22   25  4 21                  15587.7997  -0.0071  0.025  -0.0071 0.25
 699: 26  4 22   25  5 21                  15587.7997  -0.0071  0.025  -0.0071 0.25
 700: 26  5 22   25  4 21                  15587.7997  -0.0071  0.025  -0.0071 0.25
 701: 26  5 22   25  5 21                  15587.7997  -0.0071  0.025  -0.0071 0.25
 702: 19 17  2   18 16  2                  15710.5553  -0.0087  0.025  -0.0087 0.25
 703: 19 17  3   18 16  2                  15710.5553  -0.0087  0.025  -0.0087 0.25
 704: 19 17  2   18 16  3                  15710.5553  -0.0087  0.025  -0.0087 0.25
 705: 19 17  3   18 16  3                  15710.5553  -0.0087  0.025  -0.0087 0.25
 706: 27  2 25   26  2 24                  15727.3018  -0.0018  0.025  -0.0019 0.25
 707: 27  2 25   26  3 24                  15727.3018  -0.0018  0.025  -0.0019 0.25
 708: 27  3 25   26  2 24                  15727.3018  -0.0018  0.025  -0.0019 0.25
 709: 27  3 25   26  3 24                  15727.3018  -0.0018  0.025  -0.0019 0.25
 710: 19 18  1   18 17  1                  15909.7990  -0.0097  0.025  -0.0097 0.25
 711: 19 18  1   18 17  2                  15909.7990  -0.0097  0.025  -0.0097 0.25
 712: 19 18  2   18 17  1                  15909.7990  -0.0097  0.025  -0.0097 0.25
 713: 19 18  2   18 17  2                  15909.7990  -0.0097  0.025  -0.0097 0.25
 714: 20 16  5   19 15  4                  16162.3329  -0.0042  0.025  -0.0107 0.25
 715: 20 16  4   19 15  4                  16162.3329  -0.0069  0.025  -0.0107 0.25
 716: 20 16  5   19 15  5                  16162.3329  -0.0144  0.025  -0.0107 0.25
 717: 20 16  4   19 15  5                  16162.3329  -0.0171  0.025  -0.0107 0.25
 718: 20 19  1   19 18  1                  16762.5087  -0.0058  0.025  -0.0058 0.25
 719: 20 19  1   19 18  2                  16762.5087  -0.0058  0.025  -0.0058 0.25
 720: 20 19  2   19 18  1                  16762.5087  -0.0058  0.025  -0.0058 0.25
 721: 20 19  2   19 18  2                  16762.5087  -0.0058  0.025  -0.0058 0.25
 722: 20 20  0   19 19  0                  16961.3623  -0.0044  0.025  -0.0044 0.25
 723: 20 20  0   19 19  1                  16961.3623  -0.0044  0.025  -0.0044 0.25
 724: 20 20  1   19 19  0                  16961.3623  -0.0044  0.025  -0.0044 0.25
 725: 20 20  1   19 19  1                  16961.3623  -0.0044  0.025  -0.0044 0.25
-------------------------------------------------------------------------------

PARAMETERS IN FIT:

       10000            A  /MHz          426.6195(2)                          1
       20000            B  /MHz          358.4285(1)                          2
       30000            C  /MHz          281.5441(1)                          3
         200           DJ  /kHz            0.0961(3)                          4
        1100          DJK  /kHz           -0.040(2)                           5
        2000           DK  /kHz            0.070(2)                           6
       40100           d1  /kHz           -0.0269(1)                          7
       50000           d2  /kHz           -0.0030(1)                          8

 MICROWAVE AVG =       -0.000534 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.008096 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.32383         0.32383

  distinct frequency lines in fit:   474
       distinct parameters of fit:     8

 for standard errors previous errors are multiplied by:   0.326598

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

       10000            A  /MHz          426.61950(7)                         1
       20000            B  /MHz          358.42855(5)                         2
       30000            C  /MHz          281.54415(5)                         3
         200           DJ  /kHz            0.0961(1)                          4
        1100          DJK  /kHz           -0.0405(7)                          5
        2000           DK  /kHz            0.0706(6)                          6
       40100           d1  /kHz           -0.02690(5)                         7
       50000           d2  /kHz           -0.00306(3)                         8

 CORRELATION COEFFICIENTS, C.ij:

           A        B        C       -DJ      -DJK     -DK      d1       d2

A           1.0000
B          -0.0988   1.0000
```

```
C          -0.0971   0.1216   1.0000
-DJ         0.3808  -0.7049  -0.3739   1.0000
-DJK       -0.6606   0.2761   0.0909  -0.7229   1.0000
-DK         0.5004  -0.1543  -0.0116   0.5882  -0.9538   1.0000
d1          0.1751  -0.7880   0.1969   0.7193  -0.4189   0.3062   1.0000
d2         -0.2420  -0.1389   0.3216  -0.3711   0.5130  -0.5146   0.1057   1.0000

 Mean value of |C.ij|, i.ne.j =   0.3767
 Mean value of  C.ij,  i.ne.j =  -0.0698


 Worst fitting lines (obs-calc/error):

   612:   -2.4        542:   -1.5        440:   -1.5        689:   -1.4
   447:    1.1        365:    1.1        320:    1.0        401:    0.9
   667:   -0.9        160:   -0.9        254:   -0.8        343:    0.8
   524:    0.7        677:   -0.7        583:    0.7        415:    0.7
   593:   -0.7        352:    0.7        439:   -0.7        477:    0.7
   539:    0.7        471:   -0.7        509:    0.7        318:   -0.6
   121:   -0.6         13:   -0.6        529:    0.6        690:   -0.6
   476:   -0.6         59:   -0.6        594:    0.6        496:   -0.6
   547:    0.6        470:    0.6        540:    0.6        426:    0.6
   497:    0.5        402:    0.5        400:    0.5        434:    0.5
   530:    0.5        444:    0.5        548:    0.5         37:    0.5
    61:    0.5        328:    0.5        573:    0.5        170:   -0.5
   429:    0.4        458:    0.4
```

SPFIT output reformatted with PIFORM

Hexamer - 6 I

							obs	o-c	error	blends		Notes
										o-c	wt	
1:	5	2	3	4	2	2	2030.5646	0.0027	0.025			
2:	5	1	4	4	1	3	2032.4118	0.0032	0.025			
3:	4	2	2	3	0	3	2277.4760	-0.0084	0.025			
4:	6	1	6	5	1	5	2281.7088	-0.0016	0.025			
5:	6	0	6	5	0	5	2298.4214	-0.0001	0.025			
6:	6	2	5	5	2	4	2365.9806	0.0011	0.025			
7:	6	5	2	5	5	1	2388.7696	0.0068	0.025	0.0020	0.50	
8:	6	5	1	5	5	0	2388.7696	-0.0028	0.025	0.0020	0.50	
9:	6	4	3	5	4	2	2391.4746	0.0056	0.025			
10:	6	4	2	5	4	1	2392.0602	0.0021	0.025			
11:	6	3	4	5	3	3	2392.2590	0.0019	0.025			
12:	6	3	3	5	3	2	2405.5904	0.0015	0.025			
13:	6	1	5	5	1	4	2426.1214	0.0042	0.025			
14:	6	2	4	5	2	3	2447.5079	0.0037	0.025			
15:	7	0	7	6	1	6	2641.8145	0.0028	0.025			
16:	7	1	7	6	1	6	2655.5649	-0.0025	0.025			
17:	7	0	7	6	0	6	2666.2267	-0.0017	0.025			
18:	7	1	7	6	0	6	2679.9725	-0.0116	0.025			
19:	7	2	6	6	2	5	2752.5044	-0.0014	0.025			
20:	7	6	2	6	6	1	2786.5041	0.0041	0.025	0.0038	0.50	
21:	7	6	1	6	6	0	2786.5041	0.0034	0.025	0.0038	0.50	
22:	7	5	3	6	5	2	2788.9848	0.0304	0.025	0.0039	0.50	
23:	7	5	2	6	5	1	2788.9848	-0.0227	0.025	0.0039	0.50	
24:	7	3	5	6	3	4	2791.1462	0.0012	0.025			
25:	7	4	4	6	4	3	2792.8409	0.0010	0.025			
26:	7	4	3	6	4	2	2794.7657	0.0014	0.025			
27:	7	1	6	6	1	5	2811.6678	0.0038	0.025			
28:	7	3	4	6	3	3	2819.0355	0.0006	0.025			
29:	7	2	5	6	2	4	2861.6388	0.0034	0.025			
30:	14	4	10	13	6	7	2885.6978	0.0302	0.025			
31:	8	0	8	7	1	7	3020.6902	-0.0036	0.025			
32:	8	1	8	7	1	7	3028.1500	-0.0029	0.025			
33:	8	0	8	7	0	7	3034.4471	-0.0023	0.025			
34:	8	1	8	7	0	7	3041.9055	-0.0031	0.025			
35:	8	2	7	7	2	6	3135.9590	0.0002	0.025			
36:	8	7	2	7	7	1	3184.2687	0.0030	0.025	0.0030	0.50	
37:	8	7	1	7	7	0	3184.2687	0.0030	0.025	0.0030	0.50	
38:	8	6	3	7	6	2	3186.4525	0.0044	0.025			
39:	8	3	6	7	3	5	3188.4440	-0.0004	0.025			
40:	8	1	7	7	1	6	3188.5453	0.0041	0.025			
41:	8	5	4	7	5	3	3190.0761	0.0030	0.025			
42:	8	5	3	7	5	2	3190.2837	0.0008	0.025			
43:	8	4	5	7	4	4	3194.9702	0.0025	0.025			
44:	8	4	4	7	4	3	3200.0943	0.0010	0.025			
45:	8	3	5	7	3	4	3238.1793	0.0019	0.025			
46:	8	2	6	7	2	5	3270.4119	0.0054	0.025			
47:	9	1	9	8	1	8	3399.8595	-0.0028	0.025			
48:	9	0	9	8	0	8	3403.3868	-0.0027	0.025			
49:	9	1	9	8	0	8	3407.3241	0.0025	0.025			
50:	9	2	8	8	2	7	3516.4068	0.0003	0.025			
51:	9	1	8	8	1	7	3558.3686	0.0037	0.025			
52:	9	8	1	8	8	0	3582.0503	0.0030	0.025	0.0031	0.50	
53:	9	8	2	8	8	1	3582.0503	0.0030	0.025	0.0031	0.50	
54:	9	3	7	8	3	6	3583.4084	0.0020	0.025			
55:	9	7	3	8	7	2	3584.0167	-0.0228	0.025	-0.0230	0.50	
56:	9	7	2	8	7	1	3584.0167	-0.0231	0.025	-0.0230	0.50	
57:	9	6	4	8	6	3	3587.1630	0.0101	0.025	0.0005	0.50	
58:	9	6	3	8	6	2	3587.1630	-0.0091	0.025	0.0005	0.50	
59:	9	5	5	8	5	4	3592.1964	0.0023	0.025			
60:	9	5	4	8	5	3	3592.8642	0.0011	0.025			
61:	9	4	6	8	4	5	3597.4514	0.0021	0.025			

62:	9	4	5	8	4	4	3609.1635	0.0013	0.025		
63:	9	3	6	8	3	5	3660.8597	0.0028	0.025		
64:	9	2	7	8	2	6	3672.0575	0.0063	0.025		
65:	10	0	10	9	1	9	3768.9715	-0.0119	0.025		
66:	10	1	10	9	1	9	3771.0086	-0.0031	0.025		
67:	10	0	10	9	0	9	3772.9126	-0.0028	0.025		
68:	10	1	10	9	0	9	3774.9364	-0.0072	0.025		
69:	10	2	9	9	2	8	3894.1285	-0.0010	0.025		
70:	10	1	9	9	1	8	3924.3632	0.0010	0.025		
71:	10	3	8	9	3	7	3975.4336	0.0014	0.025		
72:	10	9	1	9	9	0	3979.8365	0.0003	0.025	0.0004	0.50
73:	10	9	2	9	9	1	3979.8365	0.0003	0.025	0.0004	0.50
74:	10	8	2	9	8	1	3981.6975	0.0029	0.025	0.0029	0.50
75:	10	8	3	9	8	2	3981.6975	0.0029	0.025	0.0029	0.50
76:	10	7	4	9	7	3	3984.4370	0.0027	0.025	0.0019	0.50
77:	10	7	3	9	7	2	3984.4370	0.0011	0.025	0.0019	0.50
78:	10	6	5	9	6	4	3988.7118	0.0013	0.025		
79:	10	6	4	9	6	3	3988.7829	0.0012	0.025		
80:	10	5	6	9	5	5	3995.3204	0.0017	0.025		
81:	10	5	5	9	5	4	3997.1432	0.0012	0.025		
82:	10	4	7	9	4	6	3999.6708	0.0015	0.025		
83:	10	4	6	9	4	5	4023.2511	0.0004	0.025		
84:	10	2	8	9	2	7	4065.0693	0.0068	0.025		
85:	10	3	7	9	3	6	4083.1733	0.0026	0.025		
86:	11	0	11	10	1	10	4140.8002	0.0040	0.025		
87:	11	1	11	10	1	10	4141.8206	-0.0041	0.025		
88:	11	0	11	10	0	10	4142.8205	-0.0039	0.025		
89:	11	2	10	10	2	9	4269.5670	-0.0019	0.025		
90:	11	1	10	10	1	9	4289.5694	0.0010	0.025		
91:	11	3	9	10	3	8	4364.1317	-0.0003	0.025		
92:	11	10	1	10	10	0	4377.6327	0.0051	0.025	0.0051	0.50
93:	11	10	2	10	10	1	4377.6327	0.0051	0.025	0.0051	0.50
94:	11	9	2	10	9	1	4379.3883	0.0012	0.025	0.0013	0.50
95:	11	9	3	10	9	2	4379.3883	0.0012	0.025	0.0013	0.50
96:	11	8	4	10	8	3	4381.8665	0.0013	0.025	0.0013	0.50
97:	11	8	3	10	8	2	4381.8665	0.0012	0.025	0.0013	0.50
98:	11	7	5	10	7	4	4385.5280	0.0032	0.025		
99:	11	7	4	10	7	3	4385.5282	-0.0031	0.025		
100:	11	6	6	10	6	5	4391.2101	0.0021	0.025		
101:	11	6	5	10	6	4	4391.4313	-0.0003	0.025		
102:	11	5	7	10	5	6	4399.3309	0.0017	0.025		
103:	11	4	8	10	4	7	4400.8603	0.0012	0.025		
104:	11	5	6	10	5	5	4403.7191	0.0006	0.025		
105:	11	4	7	10	4	6	4443.2276	0.0000	0.025		
106:	11	2	9	10	2	8	4448.3898	0.0076	0.025		
107:	11	3	8	10	3	7	4501.2026	0.0050	0.025		
108:	12	0	12	11	1	11	4511.9239	-0.0065	0.025		
109:	12	1	12	11	1	11	4512.4413	-0.0036	0.025		
110:	12	0	12	11	0	11	4512.9545	-0.0045	0.025		
111:	12	1	12	11	0	11	4513.4976	0.0241	0.025		
112:	12	2	11	11	2	10	4643.2351	-0.0022	0.025		
113:	12	1	11	11	1	10	4655.6256	-0.0014	0.025		
114:	12	3	10	11	3	9	4749.3569	0.0000	0.025		
115:	12	11	1	11	11	0	4775.4199	0.0017	0.025	0.0017	0.50
116:	12	11	2	11	11	1	4775.4199	0.0017	0.025	0.0017	0.50
117:	12	10	2	11	10	1	4777.1033	0.0014	0.025	0.0014	0.50
118:	12	10	3	11	10	2	4777.1033	0.0014	0.025	0.0014	0.50
119:	12	9	3	11	9	2	4779.3913	0.0020	0.025	0.0021	0.50
120:	12	9	4	11	9	3	4779.3913	0.0020	0.025	0.0021	0.50
121:	12	8	5	11	8	4	4782.6166	0.0009	0.025	0.0007	0.50
122:	12	8	4	11	8	3	4782.6166	0.0004	0.025	0.0007	0.50
123:	12	7	6	11	7	5	4787.3997	0.0114	0.025	-0.0003	0.50
124:	12	7	5	11	7	4	4787.3997	-0.0120	0.025	-0.0003	0.50
125:	12	6	6	11	6	5	4795.3281	-0.0007	0.025		
126:	12	4	9	11	4	8	4800.1989	0.0000	0.025		
127:	12	5	8	11	5	7	4803.9438	0.0009	0.025		
128:	9	3	6	8	1	7	4812.2167	0.0164	0.025		
129:	12	5	7	11	5	6	4813.4670	-0.0002	0.025		
130:	12	2	10	11	2	9	4822.2707	0.0073	0.025		
131:	12	4	8	11	4	7	4868.5481	0.0005	0.025		

132:	13	1	13	12	1	12	4882.9540	-0.0041	0.025	
133:	13	0	13	12	0	12	4883.2139	-0.0042	0.025	
134:	12	3	9	11	3	8	4912.1304	0.0070	0.025	
135:	13	2	12	12	2	11	5015.6275	-0.0035	0.025	
136:	13	3	11	12	3	10	5131.2041	0.0000	0.025	
137:	13	10	3	12	10	2	5176.9741	0.0018	0.025	0.0018 0.50
138:	13	10	4	12	10	3	5176.9741	0.0018	0.025	0.0018 0.50
139:	13	9	5	12	9	4	5179.8879	0.0012	0.025	0.0012 0.50
140:	13	9	4	12	9	3	5179.8879	0.0012	0.025	0.0012 0.50
141:	13	8	6	12	8	5	5184.0091	0.0039	0.025	0.0029 0.50
142:	13	8	5	12	8	4	5184.0091	0.0017	0.025	0.0029 0.50
143:	13	2	11	12	2	10	5188.9443	0.0071	0.025	
144:	13	7	7	12	7	6	5190.1037	0.0007	0.025	
145:	13	7	6	12	7	5	5190.1795	0.0036	0.025	
146:	13	4	10	12	4	9	5196.9295	0.0013	0.025	
147:	13	6	8	12	6	7	5199.2352	0.0008	0.025	
148:	13	6	7	12	6	6	5200.7770	0.0012	0.025	
149:	13	5	9	12	5	8	5208.6875	0.0009	0.025	
150:	13	5	8	12	5	7	5227.5313	-0.0002	0.025	
151:	14	1	14	13	1	13	5253.4106	-0.0021	0.025	
152:	14	0	14	13	0	13	5253.5402	-0.0022	0.025	
153:	13	4	9	12	4	8	5296.5305	0.0004	0.025	
154:	13	3	10	12	3	9	5314.0989	0.0089	0.025	
155:	14	2	13	13	2	12	5387.1636	-0.0052	0.025	
156:	14	1	13	13	1	12	5391.3257	-0.0033	0.025	
157:	9	3	7	8	1	8	5485.0661	-0.0005	0.025	
158:	14	3	12	13	3	11	5509.9902	-0.0006	0.025	
159:	14	2	12	13	2	11	5551.9680	0.0059	0.025	
160:	14	12	2	13	12	1	5572.5654	0.0016	0.025	0.0016 0.50
161:	14	12	3	13	12	2	5572.5654	0.0016	0.025	0.0016 0.50
162:	14	11	3	13	11	2	5574.5958	0.0024	0.025	0.0024 0.50
163:	14	11	4	13	11	3	5574.5958	0.0024	0.025	0.0024 0.50
164:	14	10	4	13	10	3	5577.2725	-0.0014	0.025	-0.0015 0.50
165:	14	10	5	13	10	4	5577.2725	-0.0014	0.025	-0.0015 0.50
166:	14	9	6	13	9	5	5580.9273	0.0023	0.025	0.0022 0.50
167:	14	9	5	13	9	4	5580.9273	0.0021	0.025	0.0022 0.50
168:	14	8	7	13	8	6	5586.0999	0.0040	0.025	0.0003 0.50
169:	14	8	6	13	8	5	5586.0999	-0.0035	0.025	0.0003 0.50
170:	14	4	11	13	4	10	5590.4433	0.0015	0.025	
171:	14	7	8	13	7	7	5593.7457	0.0022	0.025	
172:	14	7	7	13	7	6	5593.9475	0.0004	0.025	
173:	14	6	8	13	6	7	5608.2297	-0.0004	0.025	
174:	14	5	10	13	5	9	5612.9062	0.0006	0.025	
175:	15	1	15	14	1	14	5623.8327	-0.0017	0.025	
176:	15	0	15	14	0	14	5623.8917	-0.0067	0.025	
177:	14	5	9	13	5	8	5647.0809	-0.0030	0.025	
178:	14	3	11	13	3	10	5705.7823	0.0108	0.025	
179:	14	4	10	13	4	9	5722.9673	0.0022	0.025	
180:	15	2	14	14	2	13	5758.1606	-0.0057	0.025	
181:	15	1	14	14	1	13	5760.4642	-0.0044	0.025	
182:	15	3	13	14	3	12	5886.1912	-0.0019	0.025	
183:	11	3	8	10	1	9	5913.8428	0.0013	0.025	
184:	15	2	13	14	2	12	5914.5402	0.0018	0.025	
185:	15	13	2	14	13	1	5970.2982	-0.0019	0.025	-0.0019 0.50
186:	15	13	3	14	13	2	5970.2982	-0.0019	0.025	-0.0019 0.50
187:	15	12	3	14	12	2	5972.2397	0.0005	0.025	0.0006 0.50
188:	15	12	4	14	12	3	5972.2397	0.0005	0.025	0.0006 0.50
189:	15	11	4	14	11	3	5974.7454	0.0069	0.025	0.0069 0.50
190:	15	11	5	14	11	4	5974.7454	0.0069	0.025	0.0069 0.50
191:	15	10	6	14	10	5	5978.0452	0.0021	0.025	0.0022 0.50
192:	15	10	5	14	10	4	5978.0452	0.0021	0.025	0.0022 0.50
193:	15	4	12	14	4	11	5980.3547	0.0009	0.025	
194:	15	9	7	14	9	6	5982.5533	0.0013	0.025	0.0010 0.50
195:	15	9	6	14	9	5	5982.5533	0.0006	0.025	0.0010 0.50
196:	15	8	8	14	8	7	5988.9639	0.0108	0.025	-0.0008 0.50
197:	15	8	7	14	8	6	5988.9639	-0.0123	0.025	-0.0008 0.50
198:	16	1	16	15	1	15	5994.2183	-0.0182	0.025	
199:	16	0	16	15	0	15	5994.2735	0.0056	0.025	
200:	15	7	9	14	7	8	5998.3735	0.0020	0.025	
201:	15	7	8	14	7	7	5998.8896	-0.0012	0.025	

202:	15	6	10	14	6	9	6010.9740	-0.0002	0.025	
203:	15	5	11	14	5	10	6015.8189	0.0001	0.025	
204:	15	6	9	14	6	8	6018.3716	-0.0023	0.025	
205:	15	5	10	14	5	9	6072.6701	-0.0039	0.025	
206:	15	3	12	14	3	11	6086.5664	0.0124	0.025	
207:	16	2	15	15	2	14	6128.8337	-0.0078	0.025	
208:	16	1	15	15	1	14	6130.0808	-0.0068	0.025	
209:	15	4	11	14	4	10	6143.7466	0.0051	0.025	
210:	16	3	14	15	3	13	6260.3572	-0.0037	0.025	
211:	17	1	17	16	1	16	6364.6299	0.0046	0.025	-0.0029 0.50
212:	17	0	17	16	0	16	6364.6299	-0.0105	0.025	-0.0029 0.50
213:	16	4	13	15	4	12	6366.5315	-0.0001	0.025	-0.0009 0.25
214:	16	15	1	15	15	0	6366.5315	-0.0011	0.025	-0.0009 0.25
215:	16	15	1	15	15	0	6366.5315	-0.0011	0.025	-0.0009 0.25
216:	16	15	2	15	15	1	6366.5315	-0.0011	0.025	-0.0009 0.25
217:	16	13	3	15	13	2	6369.9036	0.0032	0.025	0.0032 0.50
218:	16	13	4	15	13	3	6369.9036	0.0032	0.025	0.0032 0.50
219:	16	12	4	15	12	3	6372.2570	0.0015	0.025	0.0015 0.50
220:	16	12	5	15	12	4	6372.2570	0.0015	0.025	0.0015 0.50
221:	16	11	5	15	11	4	6375.2974	0.0032	0.025	0.0032 0.50
222:	16	11	6	15	11	5	6375.2974	0.0032	0.025	0.0032 0.50
223:	16	10	7	15	10	6	6379.3173	0.0001	0.025	0.0001 0.50
224:	16	10	6	15	10	5	6379.3173	0.0001	0.025	0.0001 0.50
225:	16	9	8	15	9	7	6384.8185	0.0003	0.025	-0.0008 0.50
226:	16	9	7	15	9	6	6384.8185	-0.0020	0.025	-0.0008 0.50
227:	16	8	9	15	8	8	6392.6515	0.0073	0.025	
228:	16	8	8	15	8	7	6392.6856	-0.0240	0.025	
229:	16	7	10	15	7	9	6404.0188	-0.0004	0.025	
230:	16	7	9	15	7	8	6405.2416	-0.0033	0.025	
231:	16	5	12	15	5	11	6416.6091	-0.0003	0.025	
232:	16	6	11	15	6	10	6417.6588	-0.0013	0.025	
233:	16	6	10	15	6	9	6432.1562	-0.0054	0.025	
234:	16	3	13	15	3	12	6457.3030	0.0130	0.025	
235:	17	2	16	16	2	15	6499.3270	-0.0067	0.025	
236:	17	1	16	16	1	15	6499.9874	-0.0087	0.025	
237:	16	5	11	15	5	10	6503.2584	-0.0046	0.025	
238:	16	4	12	15	4	11	6555.9055	0.0075	0.025	
239:	17	3	15	16	3	14	6633.0277	-0.0063	0.025	
240:	17	2	15	16	2	14	6644.0239	-0.0046	0.025	
241:	18	1	18	17	1	17	6735.0049	0.0014	0.025	-0.0022 0.50
242:	18	0	18	17	0	17	6735.0049	-0.0058	0.025	-0.0022 0.50
243:	17	4	14	16	4	13	6749.0954	-0.0010	0.025	
244:	17	13	4	16	13	3	6769.8161	0.0076	0.025	0.0076 0.50
245:	17	13	5	16	13	4	6769.8161	0.0076	0.025	0.0076 0.50
246:	17	12	5	16	12	4	6772.6373	0.0000	0.025	-0.0001 0.50
247:	17	12	6	16	12	5	6772.6373	0.0000	0.025	-0.0001 0.50
248:	17	11	7	16	11	6	6776.2907	-0.0001	0.025	-0.0001 0.50
249:	17	11	6	16	11	5	6776.2907	-0.0001	0.025	-0.0001 0.50
250:	17	10	8	16	10	7	6781.1334	-0.0023	0.025	-0.0024 0.50
251:	17	10	7	16	10	6	6781.1334	-0.0025	0.025	-0.0024 0.50
252:	17	9	9	16	9	8	6787.7803	0.0031	0.025	-0.0005 0.50
253:	17	9	8	16	9	7	6787.7803	-0.0041	0.025	-0.0005 0.50
254:	17	8	10	16	8	9	6797.2356	-0.0007	0.025	
255:	17	8	9	16	8	8	6797.4024	-0.0040	0.025	
256:	17	7	11	16	7	10	6810.6628	-0.0018	0.025	
257:	17	7	10	16	7	9	6813.3579	-0.0050	0.025	
258:	17	5	13	16	5	12	6814.5275	-0.0006	0.025	
259:	17	3	14	16	3	13	6820.7609	0.0126	0.025	
260:	17	6	12	16	6	11	6824.2533	0.0000	0.025	
261:	17	6	11	16	6	10	6850.7556	-0.0078	0.025	
262:	18	2	17	17	2	16	6869.7184	-0.0081	0.025	
263:	18	1	17	17	1	16	6870.0646	-0.0088	0.025	
264:	17	5	12	16	5	11	6935.6854	-0.0051	0.025	
265:	17	4	13	16	4	12	6957.5515	0.0111	0.025	
266:	18	3	16	17	3	15	7004.6724	-0.0068	0.025	
267:	18	2	16	17	2	15	7011.1420	-0.0057	0.025	
268:	19	1	19	18	1	18	7105.3749	0.0031	0.025	0.0014 0.50
269:	19	0	19	18	0	18	7105.3749	-0.0003	0.025	0.0014 0.50
270:	18	4	15	17	4	14	7128.3879	-0.0020	0.025	
271:	18	13	6	17	13	5	7170.0403	-0.0050	0.025	

272:	18	12	6	17	12	5	7173.4056	-0.0040	0.025	-0.0040	0.50
273:	18	12	7	17	12	6	7173.4056	-0.0040	0.025	-0.0040	0.50
274:	18	11	8	17	11	7	7177.7554	-0.0046	0.025	-0.0046	0.50
275:	18	11	7	17	11	6	7177.7554	-0.0046	0.025	-0.0046	0.50
276:	18	3	15	17	3	14	7180.8125	0.0096	0.025		
277:	18	10	9	17	10	8	7183.5391	-0.0012	0.025	-0.0016	0.50
278:	18	10	8	17	10	7	7183.5391	-0.0019	0.025	-0.0016	0.50
279:	18	9	10	17	9	9	7191.4934	0.0073	0.025	-0.0030	0.50
280:	18	9	9	17	9	8	7191.4934	-0.0134	0.025	-0.0030	0.50
281:	18	8	11	17	8	10	7202.7872	-0.0030	0.025		
282:	18	8	10	17	8	9	7203.1911	-0.0112	0.025		
283:	18	5	14	17	5	13	7208.9839	-0.0006	0.025		
284:	18	7	12	17	7	11	7218.1945	-0.0023	0.025		
285:	18	7	11	17	7	10	7223.7648	-0.0087	0.025		
286:	18	6	13	17	6	12	7230.0662	-0.0035	0.025		
287:	19	2	18	18	2	17	7240.0604	-0.0069	0.025		
288:	19	1	18	18	1	17	7240.2363	-0.0103	0.025		
289:	18	6	12	17	6	11	7275.2353	-0.0113	0.025		
290:	18	4	14	17	4	13	7347.5294	0.0256	0.025		
291:	18	5	13	17	5	12	7365.4366	-0.0012	0.025		
292:	19	3	17	18	3	16	7375.6512	-0.0097	0.025		
293:	19	2	17	18	2	16	7379.3570	-0.0077	0.025		
294:	20	1	20	19	1	19	7475.7346	0.0041	0.025	0.0033	0.50
295:	20	0	20	19	0	19	7475.7346	0.0024	0.025	0.0033	0.50
296:	19	4	16	18	4	15	7504.9068	-0.0047	0.025		
297:	19	3	16	18	3	15	7540.7963	0.0060	0.025		
298:	19	13	6	18	13	5	7570.6350	0.0032	0.025	0.0032	0.50
299:	19	13	7	18	13	6	7570.6350	0.0032	0.025	0.0032	0.50
300:	19	12	7	18	12	6	7574.5880	-0.0101	0.025	-0.0102	0.50
301:	19	12	8	18	12	7	7574.5880	-0.0101	0.025	-0.0102	0.50
302:	19	11	8	18	11	7	7579.7301	-0.0048	0.025	-0.0048	0.50
303:	19	11	9	18	11	8	7579.7301	-0.0047	0.025	-0.0048	0.50
304:	19	10	10	18	10	9	7586.5731	-0.0023	0.025	-0.0035	0.50
305:	19	10	9	18	10	8	7586.5731	-0.0046	0.025	-0.0035	0.50
306:	19	5	15	18	5	14	7599.6128	-0.0001	0.025		
307:	19	8	12	18	8	11	7609.3421	-0.0066	0.025		
308:	19	8	11	18	8	10	7610.2793	-0.0073	0.025		
309:	20	2	19	19	2	18	7610.3723	-0.0088	0.025		
310:	20	1	19	19	1	18	7610.4626	-0.0102	0.025		
311:	19	7	13	18	7	12	7626.3735	-0.0061	0.025		
312:	19	6	14	18	6	13	7634.3140	-0.0040	0.025		
313:	19	7	12	18	7	11	7637.2327	-0.0102	0.025		
314:	19	6	13	18	6	12	7705.8449	-0.0138	0.025		
315:	13	4	10	12	2	11	7708.9239	0.0087	0.025		
316:	19	4	15	18	4	14	7725.5772	0.0178	0.025		
317:	20	3	18	19	3	17	7746.2285	-0.0114	0.025		
318:	20	2	18	19	2	17	7748.3035	-0.0112	0.025		
319:	19	5	14	18	5	13	7788.2295	0.0028	0.025		
320:	21	1	21	20	1	20	7846.0954	0.0163	0.025	0.0159	0.50
321:	21	0	21	20	0	20	7846.0954	0.0155	0.025	0.0159	0.50
322:	20	4	17	19	4	16	7879.2298	-0.0049	0.025		
323:	20	3	17	19	3	16	7902.5149	0.0010	0.025		
324:	20	11	10	19	11	9	7982.2378	-0.0123	0.025	-0.0125	0.50
325:	20	11	9	19	11	8	7982.2378	-0.0125	0.025	-0.0125	0.50
326:	20	5	16	19	5	15	7986.3032	-0.0013	0.025		
327:	20	10	11	19	10	10	7990.2825	-0.0062	0.025	-0.0095	0.50
328:	20	10	10	19	10	9	7990.2825	-0.0126	0.025	-0.0095	0.50
329:	20	8	13	19	8	12	8016.9212	0.0021	0.025		
330:	20	8	12	19	8	11	8018.9257	-0.0097	0.025		
331:	20	6	15	19	6	14	8036.1907	0.0049	0.025		
332:	21	3	19	20	3	18	8116.5901	0.0001	0.025		
333:	21	2	19	20	2	18	8117.7251	-0.0060	0.025		
334:	20	6	14	19	6	13	8141.0932	-0.0051	0.025		
335:	22	1	22	21	1	21	8216.4363	0.0192	0.025	0.0190	0.50
336:	22	0	22	21	0	21	8216.4363	0.0188	0.025	0.0190	0.50
337:	21	4	18	20	4	17	8251.9291	0.0039	0.025		
338:	21	3	18	20	3	17	8266.4201	0.0094	0.025		
339:	22	2	21	21	2	20	8350.9823	0.0107	0.025	-0.0009	0.50
340:	22	1	21	21	1	20	8350.9823	-0.0126	0.025	-0.0009	0.50
341:	21	14	8	20	14	7	8368.6923	-0.0002	0.025		

342:	21	5	17	20	5	16	8369.2131	0.0076	0.025		
343:	21	9	13	20	9	12	8407.7372	0.0178	0.025		
344:	21	9	12	20	9	11	8408.0331	-0.0015	0.025		
345:	21	6	16	20	6	15	8434.9379	0.0003	0.025		
346:	21	7	14	20	7	13	8477.6177	-0.0104	0.025		
347:	22	3	20	21	3	19	8486.8143	-0.0039	0.025		
348:	22	2	20	21	2	19	8487.4331	-0.0032	0.025		
349:	21	6	15	20	6	14	8577.3494	-0.0053	0.025		
350:	21	5	16	20	5	15	8601.8915	0.0245	0.025		
351:	22	4	19	21	4	18	8623.4765	-0.0025	0.025		
352:	22	3	19	21	3	18	8632.2004	-0.0026	0.025		
353:	23	2	22	22	2	21	8721.2661	0.0106	0.025	0.0048	0.50
354:	23	1	22	22	1	21	8721.2661	-0.0009	0.025	0.0048	0.50
355:	22	5	18	21	5	17	8748.6864	0.0043	0.025		
356:	22	14	8	21	14	7	8769.8162	0.0068	0.025	0.0068	0.50
357:	22	14	9	21	14	8	8769.8162	0.0068	0.025	0.0068	0.50
358:	22	13	9	21	13	8	8774.7072	-0.0012	0.025	-0.0012	0.50
359:	22	13	10	21	13	9	8774.7072	-0.0012	0.025	-0.0012	0.50
360:	22	12	10	21	12	9	8780.9362	-0.0009	0.025	-0.0010	0.50
361:	22	12	11	21	12	10	8780.9362	-0.0009	0.025	-0.0010	0.50
362:	22	11	12	21	11	11	8789.0531	-0.0002	0.025	-0.0013	0.50
363:	22	11	11	21	11	10	8789.0531	-0.0022	0.025	-0.0013	0.50
364:	22	4	18	21	4	17	8810.5194	0.0233	0.025		
365:	22	9	14	21	9	13	8815.0261	0.0025	0.025		
366:	22	9	13	21	9	12	8815.7216	-0.0009	0.025		
367:	22	6	17	21	6	16	8830.0134	0.0099	0.025		
368:	22	8	15	21	8	14	8834.7797	0.0008	0.025		
369:	23	3	21	22	3	20	8856.9808	-0.0071	0.025		
370:	23	2	21	22	2	20	8857.3086	-0.0096	0.025		
371:	22	7	15	21	7	14	8906.6612	-0.0168	0.025		
372:	24	1	24	23	1	23	8957.0834	0.0246	0.025	0.0246	0.50
373:	24	0	24	23	0	23	8957.0834	0.0245	0.025	0.0246	0.50
374:	22	5	17	21	5	16	8989.8618	0.0336	0.025		
375:	23	4	20	22	4	19	8994.2857	-0.0058	0.025		
376:	23	3	20	22	3	19	8999.4037	-0.0068	0.025		
377:	22	6	16	21	6	15	9009.8121	-0.0065	0.025		
378:	23	5	19	22	5	18	9125.2588	0.0045	0.025		
379:	23	4	19	22	4	18	9167.9886	0.0165	0.025		
380:	23	14	9	22	14	8	9171.2916	-0.0070	0.025	-0.0070	0.50
381:	23	14	10	22	14	9	9171.2916	-0.0070	0.025	-0.0070	0.50
382:	23	13	10	22	13	9	9176.9615	0.0442	0.025	0.0443	0.50
383:	23	13	11	22	13	10	9176.9615	0.0443	0.025	0.0443	0.50
384:	23	12	12	22	12	11	9184.0674	-0.0062	0.025	-0.0063	0.50
385:	23	12	11	22	12	10	9184.0674	-0.0064	0.025	-0.0063	0.50
386:	23	11	13	22	11	12	9193.4162	-0.0078	0.025	-0.0105	0.50
387:	23	11	12	22	11	11	9193.4162	-0.0132	0.025	-0.0105	0.50
388:	23	7	17	22	7	16	9255.3841	-0.0004	0.025		
389:	23	8	15	22	8	14	9259.3631	-0.0130	0.025		
390:	25	0	25	24	0	24	9327.3847	0.0233	0.025	0.0233	0.50
391:	25	1	25	24	1	24	9327.3847	0.0233	0.025	0.0233	0.50
392:	23	7	16	22	7	15	9341.8685	-0.0223	0.025		
393:	24	3	21	23	3	20	9367.5773	-0.0148	0.025		
394:	23	6	17	22	6	16	9434.0861	0.0165	0.025		
395:	26	0	26	25	0	25	9697.6845	0.0338	0.025	0.0338	0.50
396:	26	1	26	25	1	25	9697.6845	0.0338	0.025	0.0338	0.50
397:	24	5	19	23	5	18	9729.3487	0.0257	0.025		
398:	25	4	22	24	4	21	9734.7424	-0.0144	0.025		
399:	25	3	22	24	3	21	9736.3992	-0.0164	0.025		
400:	24	7	17	23	7	16	9781.2996	-0.0176	0.025		
401:	29	0	29	28	0	28	10808.4179	-0.0161	0.025	-0.0162	0.50
402:	29	1	29	28	1	28	10808.4179	-0.0161	0.025	-0.0162	0.50
403:	29	2	28	28	2	27	10942.7843	0.0000	0.025	0.0000	0.50
404:	29	1	28	28	1	27	10942.7843	-0.0001	0.025	0.0000	0.50

PARAMETERS IN FIT (values truncated and Nlines statistics):

10000	A	/MHz	356.111(2)	1
20000	B	/MHz	211.5252(1)	2
30000	C	/MHz	185.2338(1)	3

```
         200           DJ  /kHz            0.0211(2)                          4
        1100          DJK  /kHz            0.013(1)                           5
        2000           DK  /kHz            0.32(5)                            6
       40100           d1  /kHz          [ 0.]                                7
       50000           d2  /kHz           -0.00075(8)                         8

 MICROWAVE AVG =        0.000125 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.008229 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.32915         0.32915

  distinct frequency lines in fit:   328
       distinct parameters of fit:     7

                                    upper state  lower state         overall
      limits of quantum number  1:      4   29       3   28           3   29
      limits of quantum number  2:      0   15       0   15           0   15
      limits of quantum number  3:      1   29       0   28           0   29

                  frequency range:        2030        10942


 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
 (values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

       10000           A  /MHz          356.1116(7)                          1
       20000           B  /MHz          211.52526(4)                         2
       30000           C  /MHz          185.23390(5)                         3
         200          DJ  /kHz            0.02118(5)                         4
        1100         DJK  /kHz            0.0135(4)                          5
        2000          DK  /kHz            0.33(2)                            6
       40100          d1  /kHz          [ 0.]                                7
       50000          d2  /kHz           -0.00076(3)                         8

 CORRELATION COEFFICIENTS, C.ij:

          A        B        C       -DJ      -DJK     -DK      d2

A          1.0000
B          0.1489   1.0000
C         -0.2098   0.2800   1.0000
-DJ        0.4020  -0.4272  -0.7790   1.0000
-DJK      -0.2712  -0.3802   0.0283  -0.2931   1.0000
-DK       -0.9046  -0.0253   0.2122  -0.4851   0.2381   1.0000
d2        -0.2951  -0.0195   0.2382  -0.3967   0.2872   0.4412   1.0000

 Mean value of |C.ij|, i.ne.j =   0.3220
 Mean value of  C.ij,  i.ne.j =  -0.1053


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

  382:    1.8        395:    1.4        374:    1.3         30:    1.2
  397:    1.0        290:    1.0        372:    1.0        350:    1.0
  111:    1.0        228:   -1.0        390:    0.9        364:    0.9
   55:   -0.9        392:   -0.9        335:    0.8        198:   -0.7
  343:    0.7        316:    0.7        400:   -0.7        371:   -0.7
  379:    0.7        394:    0.7        399:   -0.7        128:    0.7
  401:   -0.6        320:    0.6        393:   -0.6        398:   -0.6
  314:   -0.6        234:    0.5        389:   -0.5        259:    0.5
  324:   -0.5        206:    0.5         65:   -0.5         18:   -0.5
  317:   -0.5        289:   -0.5        318:   -0.4        282:   -0.4
  265:    0.4        178:    0.4        386:   -0.4        346:   -0.4
  288:   -0.4        310:   -0.4        313:   -0.4        300:   -0.4
  367:    0.4        292:   -0.4

  382: 23 13 10   22 13  9                    9176.9615   0.0442  0.025   0.0443 0.50
  395: 26  0 26   25  0 25                    9697.6845   0.0338  0.025   0.0338 0.50
```

```
   374: 22  5 17   21  5 16                8989.8618   0.0336  0.025
    30: 14  4 10   13  6  7                2885.6978   0.0302  0.025
   397: 24  5 19   23  5 18                9729.3487   0.0257  0.025
   290: 18  4 14   17  4 13                7347.5294   0.0256  0.025
   372: 24  1 24   23  1 23                8957.0834   0.0246  0.025   0.0246 0.50
   350: 21  5 16   20  5 15                8601.8915   0.0245  0.025
   111: 12  1 12   11  0 11                4513.4976   0.0241  0.025
   228: 16  8  8   15  8  7                6392.6856  -0.0240  0.025
                                                    _____________________________
_____________________________________________/ SPFIT output reformatted with PIFORM
```

Hexamer - 6 II

							obs	o-c	error	blends o-c	blends wt	Notes
1:	5	0	5	4	0	4	2320.1607	0.0006	0.025			
2:	5	1	5	4	1	4	2319.0224	0.0008	0.025			
3:	4	4	0	3	3	0	2380.2291	0.0013	0.025			
4:	4	4	1	3	3	1	2384.8246	0.0016	0.025			
5:	5	2	4	4	2	3	2421.6726	0.0023	0.025			
6:	5	1	4	4	1	3	2443.4540	0.0014	0.025			
7:	5	3	3	4	3	2	2487.3030	0.0004	0.025			
8:	5	2	3	4	2	2	2551.8423	0.0017	0.025			
9:	5	3	2	4	3	1	2561.5284	0.0022	0.025			
10:	5	3	2	4	2	2	2766.4299	0.0007	0.025			
11:	6	1	6	5	1	5	2772.1027	0.0012	0.025			
12:	6	0	6	5	0	5	2772.3761	-0.0006	0.025			
13:	5	2	4	4	1	4	2816.1894	-0.0052	0.025			
14:	5	3	3	4	2	3	2830.6010	0.0016	0.025			
15:	5	4	1	4	3	1	2869.3147	0.0010	0.025			
16:	6	2	5	5	2	4	2881.0088	-0.0040	0.025			
17:	5	4	2	4	3	2	2892.7518	0.0002	0.025			
18:	6	3	4	5	3	3	2967.9987	0.0004	0.025			
19:	5	5	0	4	4	0	2991.4022	0.0021	0.025			
20:	5	5	1	4	4	1	2992.7231	0.0009	0.025			
21:	6	4	3	5	4	2	3006.3459	0.0020	0.025			
22:	6	2	4	5	2	3	3021.3158	0.0009	0.025			
23:	6	4	2	5	4	1	3048.7648	0.0007	0.025			
24:	6	3	3	5	3	2	3085.5278	0.0004	0.025			
25:	7	1	7	6	1	6	3224.8897	0.0047	0.025			
26:	7	0	7	6	0	6	3224.9504	0.0036	0.025			
27:	6	3	3	5	2	3	3300.1179	0.0017	0.025			
28:	7	2	6	6	2	5	3336.1150	0.0018	0.025			
29:	7	1	6	6	1	5	3338.7539	0.0007	0.025			
30:	6	2	4	5	1	4	3339.5122	-0.0020	0.025			
31:	6	4	2	5	3	2	3356.5537	0.0021	0.025			
32:	6	1	5	5	0	5	3374.9585	0.0145	0.025			
33:	6	3	4	5	2	4	3376.9246	-0.0026	0.025			
34:	6	2	5	5	1	5	3378.1931	0.0073	0.025			
35:	6	4	3	5	3	3	3411.7944	0.0016	0.025			
36:	7	3	5	6	3	4	3437.4611	0.0015	0.025			
37:	7	2	5	6	2	4	3468.1691	0.0010	0.025			
38:	6	5	1	5	4	1	3485.3921	0.0017	0.025			
39:	6	5	2	5	4	2	3495.0874	0.0005	0.025			
40:	7	4	4	6	4	3	3500.9234	0.0010	0.025			
41:	7	5	3	6	5	2	3514.9466	0.0014	0.025			
42:	7	5	2	6	5	1	3533.2162	0.0009	0.025			
43:	7	3	4	6	3	3	3584.0155	-0.0088	0.025			
44:	7	4	3	6	4	2	3590.5206	0.0012	0.025			
45:	6	6	0	5	5	0	3601.3896	0.0033	0.025			
46:	6	6	1	5	5	1	3601.7217	0.0000	0.025			
47:	8	1	8	7	1	7	3677.6040	0.0079	0.025	0.0013	0.50	
48:	8	0	8	7	0	7	3677.6040	-0.0052	0.025	0.0013	0.50	
49:	8	2	7	7	2	6	3789.4704	0.0007	0.025			
50:	8	1	7	7	1	6	3790.1890	-0.0003	0.025			
51:	7	4	3	6	3	3	3861.5444	0.0008	0.025			
52:	7	3	4	6	2	4	3862.8250	-0.0005	0.025			
53:	8	3	6	7	3	5	3898.2066	0.0003	0.025			
54:	8	2	6	7	2	5	3910.9794	-0.0007	0.025			
55:	7	2	5	6	1	5	3918.1705	0.0016	0.025			
56:	7	3	5	6	2	5	3933.3743	0.0003	0.025			
57:	7	1	6	6	0	6	3941.3211	0.0007	0.025			
58:	7	4	4	6	3	4	3944.7194	0.0024	0.025			
59:	7	5	2	6	4	2	3969.8431	0.0015	0.025			
60:	8	4	5	7	4	4	3983.8753	-0.0003	0.025			
61:	7	5	3	6	4	3	4003.6912	0.0030	0.025			
62:	8	7	2	7	7	1	4005.4857	0.0051	0.025			
63:	8	7	1	7	7	0	4005.7703	-0.0054	0.025			
64:	8	6	3	7	6	2	4017.4005	0.0036	0.025			

65:	8	5	4	7	5	3	4020.3803	0.0009	0.025		
66:	8	6	2	7	6	1	4023.8291	0.0014	0.025		
67:	8	3	5	7	3	4	4050.7207	0.0001	0.025		
68:	8	5	3	7	5	2	4073.5178	-0.0009	0.025		
69:	7	6	1	6	5	1	4098.6263	0.0022	0.025		
70:	7	6	2	6	5	2	4101.8023	0.0015	0.025		
71:	8	4	4	7	4	3	4118.5662	0.0002	0.025		
72:	9	1	9	8	1	8	4130.2941	0.0033	0.025	0.0020	0.50
73:	9	0	9	8	0	8	4130.2941	0.0006	0.025	0.0020	0.50
74:	7	7	0	6	6	0	4210.9715	0.0040	0.025		
75:	7	7	1	6	6	1	4211.0468	0.0003	0.025		
76:	9	2	8	8	2	7	4242.2736	0.0031	0.025		
77:	9	1	8	8	1	7	4242.4520	0.0009	0.025		
78:	9	3	7	8	3	6	4353.8897	0.0002	0.025		
79:	9	2	7	8	2	6	4358.1846	-0.0004	0.025		
80:	8	4	4	7	3	4	4396.0872	0.0020	0.025		
81:	8	3	5	7	2	5	4445.3789	0.0008	0.025		
82:	8	5	3	7	4	3	4452.8397	-0.0012	0.025		
83:	9	4	6	8	4	5	4454.8550	0.0000	0.025		
84:	8	2	6	7	1	6	4490.3971	0.0012	0.025		
85:	8	4	5	7	3	5	4491.1334	0.0003	0.025		
86:	9	3	6	8	3	5	4493.8325	0.0004	0.025		
87:	8	3	6	7	2	6	4495.4676	0.0004	0.025		
88:	8	1	7	7	0	7	4506.5685	0.0055	0.025		
89:	8	2	7	7	1	7	4506.7792	-0.0029	0.025		
90:	9	5	5	8	5	4	4517.0882	0.0015	0.025		
91:	8	5	4	7	4	4	4523.1460	0.0007	0.025		
92:	9	6	3	8	6	2	4553.3473	-0.0006	0.025		
93:	10	1	10	9	1	9	4582.9814	0.0010	0.025	0.0008	0.50
94:	10	0	10	9	0	9	4582.9814	0.0004	0.025	0.0008	0.50
95:	8	6	2	7	5	2	4589.2366	0.0001	0.025		
96:	8	6	3	7	5	3	4604.2528	0.0004	0.025		
97:	9	4	5	8	4	4	4617.1250	-0.0008	0.025		
98:	9	5	4	8	5	3	4621.3470	0.0006	0.025		
99:	10	2	9	9	2	8	4694.9414	0.0082	0.025		
100:	10	1	9	9	1	8	4694.9748	-0.0012	0.025		
101:	8	7	1	7	6	1	4709.5067	0.0011	0.025		
102:	8	7	2	7	6	2	4710.4175	0.0015	0.025		
103:	8	5	3	7	3	4	4730.3574	-0.0028	0.025		
104:	10	3	8	9	3	7	4807.3441	-0.0051	0.025		
105:	10	2	8	9	2	7	4808.6180	-0.0014	0.025		
106:	8	8	0	7	7	0	4820.4389	0.0098	0.025	0.0010	0.50
107:	8	8	1	7	7	1	4820.4389	-0.0078	0.025	0.0010	0.50
108:	10	4	7	9	4	6	4916.4417	-0.0004	0.025		
109:	10	3	7	9	3	6	4933.3681	-0.0009	0.025		
110:	9	5	4	8	4	4	4955.6221	0.0007	0.025		
111:	9	4	5	8	3	5	4962.4940	0.0034	0.025		
112:	10	5	6	9	5	5	5001.5710	-0.0012	0.025		
113:	10	8	3	9	8	2	5015.9749	0.0005	0.025		
114:	10	8	2	9	8	1	5016.5391	-0.0034	0.025		
115:	9	3	6	8	2	6	5028.2363	0.0063	0.025		
116:	10	7	4	9	7	3	5031.3323	0.0120	0.025		
117:	11	1	11	10	1	10	5035.6688	0.0024	0.025	0.0024	0.50
118:	11	0	11	10	0	10	5035.6688	0.0023	0.025	0.0024	0.50
119:	10	6	5	9	6	4	5036.7621	0.0000	0.025		
120:	10	7	3	9	7	2	5040.4025	0.0039	0.025		
121:	9	4	6	8	3	6	5047.7834	0.0015	0.025		
122:	9	5	5	8	4	5	5056.3559	-0.0002	0.025		
123:	9	2	7	8	1	7	5058.3921	0.0004	0.025		
124:	9	3	7	8	2	7	5059.8856	-0.0014	0.025		
125:	9	6	3	8	5	3	5069.0652	-0.0003	0.025		
126:	10	4	6	9	4	5	5080.9131	-0.0031	0.025		
127:	10	6	4	9	6	3	5100.3243	-0.0004	0.025		
128:	9	6	4	8	5	4	5113.0120	0.0006	0.025		
129:	11	2	10	10	2	9	5147.5806	0.0067	0.025	0.0019	0.50
130:	11	1	10	10	1	9	5147.5806	-0.0030	0.025	0.0019	0.50
131:	10	5	5	9	5	4	5152.6339	0.0000	0.025		
132:	9	7	2	8	6	2	5204.7952	0.0010	0.025		
133:	9	7	3	8	6	3	5210.1421	0.0007	0.025		
134:	11	3	9	10	3	8	5260.0647	0.0019	0.025		

135:	11	2	9	10	2	8	5260.4068	-0.0009	0.025		
136:	9	5	4	8	3	5	5300.9849	-0.0011	0.025		
137:	9	8	1	8	7	1	5319.4331	0.0040	0.025		
138:	9	8	2	8	7	2	5319.6671	-0.0018	0.025		
139:	11	4	8	10	4	7	5372.4103	-0.0002	0.025		
140:	11	3	8	10	3	7	5378.4292	-0.0012	0.025		
141:	9	9	0	8	8	0	5429.8556	0.0039	0.025	0.0021	0.50
142:	9	9	1	8	8	1	5429.8556	0.0001	0.025	0.0021	0.50
143:	11	5	7	10	5	6	5473.5297	-0.0020	0.025		
144:	12	0	12	11	0	11	5488.3518	0.0039	0.025	0.0039	0.50
145:	12	1	12	11	1	11	5488.3518	0.0039	0.025	0.0039	0.50
146:	10	5	5	9	4	5	5491.1316	0.0022	0.025		
147:	11	4	7	10	4	6	5520.2642	-0.0032	0.025		
148:	11	8	4	10	8	3	5530.4543	0.0015	0.025		
149:	11	8	3	10	8	2	5533.4544	0.0001	0.025		
150:	11	7	5	10	7	4	5545.4505	-0.0023	0.025		
151:	10	6	4	9	5	4	5548.0445	0.0005	0.025		
152:	10	4	6	9	3	6	5549.5757	0.0009	0.025		
153:	11	7	4	10	7	3	5575.6416	-0.0004	0.025		
154:	12	2	11	11	2	10	5600.2198	0.0030	0.025	0.0020	0.50
155:	12	1	11	11	1	10	5600.2198	0.0009	0.025	0.0020	0.50
156:	10	5	6	9	4	6	5603.0738	0.0003	0.025		
157:	10	3	7	9	2	7	5603.4145	0.0005	0.025		
158:	10	4	7	9	3	7	5610.3349	0.0002	0.025		
159:	10	2	8	9	1	8	5624.5629	0.0029	0.025		
160:	10	3	8	9	2	8	5624.9617	-0.0042	0.025		
161:	10	6	5	9	5	5	5632.6866	-0.0001	0.025		
162:	10	1	9	9	0	9	5636.0950	0.0077	0.025	0.0018	0.50
163:	10	2	9	9	1	9	5636.0950	-0.0040	0.025	0.0018	0.50
164:	11	5	6	10	5	5	5650.8918	-0.0001	0.025		
165:	11	6	5	10	6	4	5653.4929	-0.0008	0.025		
166:	10	7	3	9	6	3	5691.8454	0.0005	0.025		
167:	10	7	4	9	6	4	5712.3229	-0.0002	0.025		
168:	12	3	10	11	3	9	5712.6003	0.0032	0.025		
169:	12	2	10	11	2	9	5712.6876	0.0024	0.025		
170:	10	8	2	9	7	2	5816.8558	0.0005	0.025		
171:	10	8	3	9	7	3	5818.5209	-0.0001	0.025		
172:	12	4	9	11	4	8	5825.8135	-0.0009	0.025		
173:	12	3	9	11	3	8	5827.6996	-0.0039	0.025		
174:	10	6	4	9	4	5	5886.5344	-0.0050	0.025		
175:	10	9	1	9	8	1	5929.0417	0.0178	0.025	-0.0119	0.50
176:	10	9	2	9	8	2	5929.0417	-0.0417	0.025	-0.0119	0.50
177:	12	5	8	11	5	7	5935.5990	-0.0006	0.025		
178:	13	0	13	12	0	12	5941.0288	0.0045	0.025	0.0045	0.50
179:	13	1	13	12	1	12	5941.0288	0.0045	0.025	0.0045	0.50
180:	12	4	8	11	4	7	5956.5449	-0.0016	0.025		
181:	10	5	5	9	3	6	5959.7955	0.0076	0.025		
182:	12	10	3	11	10	2	6013.4735	0.0053	0.025	-0.0141	0.50
183:	12	10	2	11	10	1	6013.4735	-0.0335	0.025	-0.0141	0.50
184:	12	6	7	11	6	6	6020.6576	0.0002	0.025		
185:	12	9	4	11	9	3	6028.5967	0.0012	0.025		
186:	12	9	3	11	9	2	6029.5045	-0.0018	0.025		
187:	10	10	0	9	9	0	6039.2583	0.0025	0.025	0.0021	0.50
188:	10	10	1	9	9	1	6039.2583	0.0017	0.025	0.0021	0.50
189:	12	8	5	11	8	4	6047.1929	-0.0015	0.025		
190:	11	6	5	10	5	5	6048.9041	0.0003	0.025		
191:	13	2	12	12	2	11	6052.8662	0.0029	0.025	0.0027	0.50
192:	13	1	12	12	1	11	6052.8662	0.0024	0.025	0.0027	0.50
193:	12	7	6	11	7	5	6054.8837	-0.0002	0.025		
194:	12	8	4	11	8	3	6059.0696	-0.0013	0.025		
195:	11	5	6	10	4	6	6061.1051	0.0000	0.025		
196:	12	5	7	11	5	6	6111.7065	-0.0021	0.025		
197:	12	7	5	11	7	4	6128.6890	0.0037	0.025		
198:	11	4	7	10	3	7	6136.4740	0.0007	0.025		
199:	11	5	7	10	4	7	6160.1627	-0.0003	0.025		
200:	13	3	11	12	3	10	6165.1313	0.0115	0.025	0.0008	0.50
201:	13	2	11	12	2	10	6165.1313	-0.0099	0.025	0.0008	0.50
202:	11	6	6	10	5	6	6166.1935	-0.0001	0.025		
203:	11	7	4	10	6	4	6167.1615	-0.0006	0.025		
204:	11	3	8	10	2	8	6173.2250	0.0000	0.025		

205:	11	4	8	10	3	8	6175.3950	-0.0008	0.025		
206:	12	6	6	11	6	5	6187.4685	-0.0007	0.025		
207:	11	2	9	10	1	9	6190.0000	0.0082	0.025		
208:	11	3	9	10	2	9	6190.0836	-0.0118	0.025		
209:	11	1	10	10	0	10	6200.6950	0.0050	0.025	0.0038	0.50
210:	11	2	10	10	1	10	6200.6950	0.0025	0.025	0.0038	0.50
211:	11	7	5	10	6	5	6221.0133	-0.0008	0.025		
212:	13	4	10	12	4	9	6278.3325	-0.0031	0.025		
213:	13	3	10	12	3	9	6278.8756	-0.0048	0.025		
214:	11	8	3	10	7	3	6309.9112	0.0002	0.025		
215:	11	8	4	10	7	4	6317.6515	-0.0020	0.025		
216:	13	5	9	12	5	8	6391.6375	-0.0014	0.025		
217:	14	0	14	13	0	13	6393.6992	0.0044	0.025	0.0044	0.50
218:	14	1	14	13	1	13	6393.6992	0.0044	0.025	0.0044	0.50
219:	11	9	2	10	8	2	6427.3194	0.0001	0.025		
220:	11	9	3	10	8	3	6427.7946	-0.0001	0.025		
221:	11	6	5	10	4	6	6459.1185	0.0015	0.025		
222:	13	6	8	12	6	7	6493.2501	-0.0026	0.025		
223:	14	2	13	13	2	12	6505.5126	0.0017	0.025	0.0017	0.50
224:	14	1	13	13	1	12	6505.5126	0.0016	0.025	0.0017	0.50
225:	13	11	3	12	11	2	6512.3558	0.0037	0.025	-0.0010	0.50
226:	13	11	2	12	11	1	6512.3558	-0.0058	0.025	-0.0010	0.50
227:	13	10	4	12	10	3	6526.6295	0.0055	0.025		
228:	13	10	3	12	10	2	6526.8797	-0.0038	0.025		
229:	11	10	1	10	9	1	6538.5101	0.0084	0.025	0.0013	0.50
230:	11	10	2	10	9	2	6538.5101	-0.0057	0.025	0.0013	0.50
231:	13	9	5	12	9	4	6545.6095	-0.0011	0.025		
232:	13	5	8	12	5	7	6547.3236	-0.0031	0.025		
233:	13	9	4	12	9	3	6549.7336	-0.0037	0.025		
234:	13	7	7	12	7	6	6554.4669	-0.0029	0.025		
235:	13	8	6	12	8	5	6563.3956	-0.0033	0.025		
236:	12	6	6	11	5	6	6585.4848	0.0036	0.025		
237:	13	8	5	12	8	4	6599.6202	-0.0030	0.025		
238:	14	3	12	13	3	11	6617.6682	0.0030	0.025	0.0006	0.50
239:	14	2	12	13	2	11	6617.6682	-0.0019	0.025	0.0006	0.50
240:	12	7	5	11	6	5	6642.3549	0.0012	0.025		
241:	11	11	0	10	10	0	6648.6463	-0.0001	0.025	-0.0002	0.50
242:	11	11	1	10	10	1	6648.6463	-0.0002	0.025	-0.0002	0.50
243:	12	5	7	11	4	7	6652.5470	0.0008	0.025		
244:	13	6	7	12	6	6	6685.1621	0.0018	0.025		
245:	12	6	7	11	5	7	6713.3186	-0.0006	0.025		
246:	12	4	8	11	3	8	6714.5902	0.0008	0.025		
247:	14	4	11	13	4	10	6730.6650	0.0055	0.025		
248:	14	3	11	13	3	10	6730.8030	-0.0040	0.025		
249:	12	3	9	11	2	9	6740.5195	-0.0014	0.025		
250:	12	7	6	11	6	6	6740.8170	-0.0019	0.025		
251:	12	4	9	11	3	9	6741.1435	-0.0039	0.025		
252:	12	2	10	11	1	10	6755.1028	0.0095	0.025	-0.0031	0.50
253:	12	3	10	11	2	10	6755.1028	-0.0157	0.025	-0.0031	0.50
254:	12	1	11	11	0	11	6765.2378	-0.0046	0.025	-0.0049	0.50
255:	12	2	11	11	1	11	6765.2378	-0.0051	0.025	-0.0049	0.50
256:	12	8	4	11	7	4	6793.3394	-0.0005	0.025		
257:	12	8	5	11	7	5	6819.3931	-0.0019	0.025		
258:	14	5	10	13	5	9	6844.8573	-0.0017	0.025		
259:	15	0	15	14	0	14	6846.3628	0.0040	0.025	0.0041	0.50
260:	15	1	15	14	1	14	6846.3628	0.0040	0.025	0.0041	0.50
261:	14	4	10	13	4	9	6847.4067	-0.0057	0.025		
262:	12	9	3	11	8	3	6923.3720	0.0006	0.025		
263:	12	9	4	11	8	4	6925.9303	-0.0072	0.025		
264:	14	6	9	13	6	8	6955.5510	-0.0059	0.025		
265:	15	1	14	14	1	13	6958.1455	-0.0115	0.025	-0.0116	0.50
266:	15	2	14	14	2	13	6958.1455	-0.0115	0.025	-0.0116	0.50
267:	14	5	9	13	5	8	6980.3858	-0.0044	0.025		
268:	12	10	2	11	9	2	7037.1438	-0.0269	0.025		
269:	12	10	3	11	9	3	7037.2981	-0.0001	0.025		
270:	14	7	8	13	7	7	7040.8519	0.0049	0.025		
271:	14	10	5	13	10	4	7042.9360	0.0000	0.025		
272:	14	10	4	13	10	3	7044.2443	-0.0081	0.025		
273:	14	9	6	13	9	5	7064.6176	0.0019	0.025		
274:	15	3	13	14	3	12	7070.2325	0.0004	0.025	-0.0001	0.50

275:	15	2	13	14	2	12	7070.2325	-0.0006	0.025	-0.0001	0.50
276:	14	8	7	13	8	6	7074.3610	-0.0019	0.025		
277:	14	9	5	13	9	4	7079.4231	0.0007	0.025		
278:	13	7	6	12	6	6	7141.5423	0.0004	0.025		
279:	14	6	8	13	6	7	7142.9588	-0.0036	0.025		
280:	12	11	1	11	10	1	7147.9300	0.0014	0.025	-0.0002	0.50
281:	12	11	2	11	10	2	7147.9300	-0.0018	0.025	-0.0002	0.50
282:	14	8	6	13	8	5	7158.2806	-0.0023	0.025		
283:	14	7	7	13	7	6	7222.9021	-0.0011	0.025		
284:	13	5	8	12	4	8	7243.3256	-0.0007	0.025		
285:	12	12	0	11	11	0	7258.0248	0.0004	0.025	0.0004	0.50
286:	12	12	1	11	11	1	7258.0248	0.0004	0.025	0.0004	0.50
287:	13	8	5	12	7	5	7264.2770	-0.0009	0.025		
288:	13	6	8	12	5	8	7270.9703	-0.0020	0.025		
289:	13	7	7	12	6	7	7274.6296	-0.0018	0.025		
290:	13	4	9	12	3	9	7286.2950	0.0002	0.025		
291:	13	5	9	12	4	9	7289.1758	-0.0008	0.025		
292:	15	5	11	14	5	10	7297.0941	-0.0042	0.025		
293:	15	4	11	14	4	10	7297.8541	-0.0162	0.025		
294:	16	0	16	15	0	15	7299.0191	0.0036	0.025	0.0036	0.50
295:	16	1	16	15	1	15	7299.0191	0.0036	0.025	0.0036	0.50
296:	13	3	10	12	2	10	7306.7267	0.0105	0.025		
297:	13	4	10	12	3	10	7306.8820	-0.0041	0.025		
298:	13	2	11	12	1	11	7320.0222	0.0065	0.025	0.0036	0.50
299:	13	3	11	12	2	11	7320.0222	0.0006	0.025	0.0036	0.50
300:	13	8	6	12	7	6	7327.9075	-0.0024	0.025		
301:	13	1	12	12	0	12	7329.7536	-0.0047	0.025	-0.0048	0.50
302:	13	2	12	12	1	12	7329.7536	-0.0048	0.025	-0.0048	0.50
303:	16	1	15	15	1	14	7410.7998	0.0002	0.025	0.0002	0.50
304:	16	2	15	15	2	14	7410.7998	0.0002	0.025	0.0002	0.50
305:	15	6	10	14	6	9	7411.5068	-0.0042	0.025		
306:	13	9	4	12	8	4	7414.0352	-0.0024	0.025		
307:	15	5	10	14	5	9	7421.0248	-0.0086	0.025		
308:	13	9	5	12	8	5	7424.3484	-0.0052	0.025		
309:	15	7	9	14	7	8	7513.8336	-0.0076	0.025		
310:	16	3	14	15	3	13	7522.8116	-0.0019	0.025	-0.0021	0.50
311:	16	2	14	15	2	13	7522.8116	-0.0022	0.025	-0.0021	0.50
312:	13	10	3	12	9	3	7534.5437	-0.0041	0.025		
313:	15	10	6	14	10	5	7562.2526	0.0006	0.025		
314:	15	10	5	14	10	4	7567.5995	-0.0078	0.025		
315:	15	9	7	14	9	6	7582.6461	-0.0033	0.025		
316:	15	9	6	14	9	5	7624.9719	-0.0019	0.025		
317:	16	4	13	15	4	12	7635.3907	0.0011	0.025	-0.0036	0.50
318:	16	3	13	15	3	12	7635.3907	-0.0083	0.025	-0.0036	0.50
319:	13	11	2	12	10	2	7646.7885	0.0053	0.025	-0.0110	0.50
320:	13	11	3	12	10	3	7646.7885	-0.0273	0.025	-0.0110	0.50
321:	14	7	7	13	6	7	7679.2835	-0.0014	0.025		
322:	15	7	8	14	7	7	7719.8130	-0.0055	0.025		
323:	15	8	7	14	8	6	7720.6351	-0.0028	0.025		
324:	14	8	6	13	7	6	7735.9018	-0.0015	0.025		
325:	16	5	12	15	5	11	7749.1441	0.0051	0.025		
326:	16	4	12	15	4	11	7749.3449	-0.0134	0.025		
327:	17	0	17	16	0	16	7751.6657	0.0011	0.025	0.0012	0.50
328:	17	1	17	16	1	16	7751.6657	0.0011	0.025	0.0012	0.50
329:	14	6	8	13	5	8	7754.5669	-0.0014	0.025		
330:	13	12	1	12	11	1	7757.3254	0.0001	0.025	-0.0002	0.50
331:	13	12	2	12	11	2	7757.3254	-0.0005	0.025	-0.0002	0.50
332:	14	7	8	13	6	8	7822.2220	-0.0036	0.025		
333:	14	5	9	13	4	9	7824.3089	0.0012	0.025		
334:	14	6	9	13	5	9	7834.8867	-0.0037	0.025		
335:	14	8	7	13	7	7	7847.8005	-0.0026	0.025		
336:	14	4	10	13	3	10	7854.8241	-0.0027	0.025		
337:	14	5	10	13	4	10	7855.6986	-0.0013	0.025		
338:	17	1	16	16	1	15	7863.4321	-0.0049	0.025	-0.0049	0.50
339:	17	2	16	16	2	15	7863.4321	-0.0049	0.025	-0.0049	0.50
340:	16	6	11	15	6	10	7864.4446	-0.0029	0.025		
341:	13	13	0	12	12	0	7867.3892	0.0000	0.025	0.0000	0.50
342:	13	13	1	12	12	1	7867.3892	0.0000	0.025	0.0000	0.50
343:	16	5	11	15	5	10	7867.6866	-0.0083	0.025		
344:	14	2	12	13	1	12	7884.8148	-0.0072	0.025	-0.0080	0.50

345:	14	3	12	13	2	12	7884.8148	-0.0086	0.025	-0.0080	0.50
346:	14	9	5	13	8	5	7893.8325	-0.0042	0.025		
347:	14	9	6	13	8	6	7925.5667	-0.0038	0.025		
348:	17	3	15	16	3	14	7975.4054	0.0022	0.025	0.0023	0.50
349:	17	2	15	16	2	14	7975.4054	0.0022	0.025	0.0023	0.50
350:	16	7	10	15	7	9	7976.2153	0.0076	0.025		
351:	16	6	10	15	6	9	8004.7972	0.0007	0.025		
352:	14	10	5	13	9	5	8032.6533	0.0010	0.025		
353:	16	10	7	15	10	6	8083.3055	0.0045	0.025		
354:	17	4	14	16	4	13	8087.8421	0.0104	0.025	0.0093	0.50
355:	17	3	14	16	3	13	8087.8421	0.0081	0.025	0.0093	0.50
356:	16	9	8	15	9	7	8094.9449	0.0066	0.025		
357:	16	10	6	15	10	5	8101.1607	0.0033	0.025		
358:	14	11	3	13	10	3	8144.7810	0.0056	0.025		
359:	14	11	4	13	10	4	8144.9950	-0.0021	0.025		
360:	17	5	13	16	5	12	8201.2679	0.0382	0.025	0.0086	0.50
361:	17	4	13	16	4	12	8201.2679	-0.0210	0.025	0.0086	0.50
362:	18	0	18	17	0	17	8204.3187	0.0133	0.025	0.0134	0.50
363:	18	1	18	17	1	17	8204.3187	0.0133	0.025	0.0134	0.50
364:	15	8	7	14	7	7	8233.6495	0.0115	0.025		
365:	15	7	8	14	6	8	8256.1508	0.0097	0.025		
366:	14	12	2	13	11	2	8256.2987	0.0118	0.025	0.0078	0.50
367:	14	12	3	13	11	3	8256.2987	0.0037	0.025	0.0078	0.50
368:	18	1	17	17	1	16	8316.0768	0.0086	0.025	0.0086	0.50
369:	18	2	17	17	2	16	8316.0768	0.0086	0.025	0.0086	0.50
370:	17	6	12	16	6	11	8316.3317	-0.0003	0.025		
371:	17	5	12	16	5	11	8317.3512	-0.0013	0.025		
372:	15	6	9	14	5	9	8349.0793	0.0083	0.025		
373:	15	9	6	14	8	6	8360.5109	-0.0167	0.025		
374:	14	13	1	13	12	1	8366.7030	0.0045	0.025	0.0045	0.50
375:	14	13	2	13	12	2	8366.7030	0.0044	0.025	0.0045	0.50
376:	15	7	9	14	6	9	8380.5146	0.0048	0.025		
377:	15	8	8	14	7	8	8381.9391	0.0081	0.025		
378:	15	5	10	14	4	10	8397.9352	0.0066	0.025		
379:	15	6	10	14	5	10	8401.5421	-0.0004	0.025		
380:	17	7	11	16	7	10	8431.9546	-0.0054	0.025		
381:	15	9	7	14	8	7	8433.8642	0.0072	0.025		
382:	15	3	12	14	2	12	8437.7563	0.0096	0.025	0.0042	0.50
383:	15	4	12	14	3	12	8437.7563	-0.0012	0.025	0.0042	0.50
384:	17	6	11	16	6	10	8443.2262	0.0040	0.025		
385:	15	2	13	14	1	13	8449.5441	-0.0001	0.025	-0.0003	0.50
386:	15	3	13	14	2	13	8449.5441	-0.0004	0.025	-0.0003	0.50
387:	15	10	5	14	9	5	8517.2550	0.0069	0.025		
388:	17	14	4	16	14	3	8520.3672	0.0067	0.025	0.0062	0.50
389:	17	14	3	16	14	2	8520.3672	0.0056	0.025	0.0062	0.50
390:	17	11	6	16	11	5	8586.7616	-0.0425	0.025		
391:	17	9	9	16	9	8	8596.3881	-0.0056	0.025		
392:	17	7	10	16	7	9	8602.8826	0.0095	0.025		
393:	15	11	4	14	10	4	8641.0991	0.0058	0.025		
394:	15	11	5	14	10	5	8642.2387	0.0013	0.025		
395:	17	10	7	16	10	6	8651.4667	-0.0016	0.025		
396:	17	8	9	16	8	8	8754.7884	0.0047	0.025		
397:	17	9	8	16	9	7	8755.2959	0.0019	0.025		
398:	18	5	13	17	5	12	8768.3451	0.0151	0.025		
399:	19	1	18	18	1	17	8768.6891	-0.0027	0.025	-0.0027	0.50
400:	19	2	18	18	2	17	8768.6891	-0.0027	0.025	-0.0027	0.50
401:	16	9	7	15	8	7	8828.7923	0.0028	0.025		
402:	15	13	2	14	12	2	8865.7337	0.0055	0.025	0.0046	0.50
403:	15	13	3	14	12	3	8865.7337	0.0036	0.025	0.0046	0.50
404:	19	2	17	18	2	16	8880.5845	-0.0042	0.025	-0.0043	0.50
405:	19	3	17	18	3	16	8880.5845	-0.0042	0.025	-0.0043	0.50
406:	18	6	12	17	6	11	8888.5001	0.0048	0.025		
407:	16	7	10	15	6	10	8945.2231	0.0167	0.025		
408:	16	5	11	15	4	11	8967.7507	-0.0024	0.025		
409:	16	6	11	15	5	11	8968.8906	-0.0011	0.025		
410:	15	14	1	14	13	1	8976.0499	-0.0010	0.025	-0.0011	0.50
411:	15	14	2	14	13	2	8976.0499	-0.0010	0.025	-0.0011	0.50
412:	19	4	16	18	4	15	8992.8123	0.0006	0.025	0.0006	0.50
413:	19	3	16	18	3	15	8992.8123	0.0004	0.025	0.0006	0.50
414:	16	10	6	15	9	6	8993.4321	0.0004	0.025		

415:	16	3	13	15	2	13	9002.9134	0.0010	0.025	-0.0003	0.50
416:	16	4	13	15	3	13	9002.9134	-0.0015	0.025	-0.0003	0.50
417:	16	2	14	15	1	14	9014.1955	-0.0055	0.025	-0.0056	0.50
418:	16	3	14	15	2	14	9014.1955	-0.0056	0.025	-0.0056	0.50
419:	18	15	4	17	15	3	9019.1110	0.0046	0.025	0.0045	0.50
420:	18	15	3	17	15	2	9019.1110	0.0043	0.025	0.0045	0.50
421:	18	9	10	17	9	9	9083.7951	0.0050	0.025		
422:	18	11	8	17	11	7	9103.0441	0.0020	0.025		
423:	19	5	15	18	5	14	9105.7295	0.0391	0.025	0.0372	0.50
424:	19	4	15	18	4	14	9105.7295	0.0353	0.025	0.0372	0.50
425:	20	0	20	19	0	19	9109.5754	0.0156	0.025	0.0157	0.50
426:	20	1	20	19	1	19	9109.5754	0.0156	0.025	0.0157	0.50
427:	18	10	9	17	10	8	9116.4310	0.0089	0.025		
428:	16	11	5	15	10	5	9133.9706	0.0061	0.025		
429:	16	11	6	15	10	6	9138.6815	-0.0029	0.025		
430:	20	1	19	19	1	18	9221.3122	0.0048	0.025	0.0049	0.50
431:	20	2	19	19	2	18	9221.3122	0.0048	0.025	0.0049	0.50
432:	18	9	9	17	9	8	9295.1198	-0.0080	0.025		
433:	20	2	18	19	2	17	9333.1832	0.0046	0.025	0.0047	0.50
434:	20	3	18	19	3	17	9333.1832	0.0046	0.025	0.0047	0.50
435:	16	13	3	15	12	3	9364.2475	0.0023	0.025	-0.0054	0.50
436:	16	13	4	15	12	4	9364.2475	-0.0132	0.025	-0.0054	0.50
437:	16	14	2	15	13	2	9475.1324	0.0067	0.025	0.0065	0.50
438:	16	14	3	15	13	3	9475.1324	0.0063	0.025	0.0065	0.50
439:	17	10	8	16	9	8	9538.9812	0.0070	0.025		
440:	20	5	16	19	5	15	9558.0305	0.0031	0.025	0.0027	0.50
441:	20	4	16	19	4	15	9558.0305	0.0022	0.025	0.0027	0.50
442:	21	0	21	20	0	20	9562.1170	-0.0554	0.025	-0.0554	0.50
443:	21	1	21	20	1	20	9562.1170	-0.0554	0.025	-0.0554	0.50
444:	16	15	1	15	14	1	9585.3835	-0.0004	0.025	-0.0004	0.50
445:	16	15	2	15	14	2	9585.3835	-0.0004	0.025	-0.0004	0.50
446:	17	11	6	16	10	6	9619.6154	0.0042	0.025		
447:	16	16	0	15	15	0	9695.3994	0.0009	0.025	0.0009	0.50
448:	16	16	1	15	15	1	9695.3994	0.0009	0.025	0.0009	0.50
449:	21	2	19	20	2	18	9785.7718	0.0083	0.025	0.0084	0.50
450:	21	3	19	20	3	18	9785.7718	0.0083	0.025	0.0084	0.50
451:	17	16	1	16	15	1	10194.6963	-0.0010	0.025	-0.0010	0.50
452:	17	16	2	16	15	2	10194.6963	-0.0010	0.025	-0.0010	0.50
453:	17	17	0	16	16	0	10304.7035	-0.0001	0.025	-0.0001	0.50
454:	17	17	1	16	16	1	10304.7035	-0.0001	0.025	-0.0001	0.50
455:	23	0	23	22	0	22	10467.3838	0.0177	0.025	0.0178	0.50
456:	23	1	23	22	1	22	10467.3838	0.0177	0.025	0.0178	0.50
457:	23	2	21	22	2	20	10690.8926	-0.0197	0.025	-0.0198	0.50
458:	23	3	21	22	3	20	10690.8926	-0.0197	0.025	-0.0198	0.50
459:	18	16	2	17	15	2	10693.8140	-0.0056	0.025	-0.0056	0.50
460:	18	16	3	17	15	3	10693.8140	-0.0056	0.025	-0.0056	0.50
461:	19	3	16	18	2	16	10697.6512	-0.0040	0.025	-0.0040	0.50
462:	19	4	16	18	3	16	10697.6512	-0.0040	0.025	-0.0040	0.50

PARAMETERS IN FIT:

10000	A	/MHz	304.7204(2)	1
20000	B	/MHz	266.1777(2)	2
30000	C	/MHz	226.3591(2)	3
200	DJ	/kHz	0.0207(4)	4
1100	DJK	/kHz	0.058(2)	5
2000	DK	/kHz	-0.037(2)	6
40100	d1	/kHz	-0.0017(2)	7
50000	d2	/kHz	-0.0017(1)	8

MICROWAVE AVG = 0.000085 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.006228 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.24911 0.24911

distinct frequency lines in fit: 385
distinct parameters of fit: 8

for standard errors previous errors are multiplied by: 0.251739

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

10000	A	/MHz	304.72043(7)	1
20000	B	/MHz	266.17778(5)	2
30000	C	/MHz	226.35912(5)	3
200	DJ	/kHz	0.0207(1)	4
1100	DJK	/kHz	0.0580(5)	5
2000	DK	/kHz	-0.0374(5)	6
40100	d1	/kHz	-0.00175(5)	7
50000	d2	/kHz	-0.00173(3)	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DJ	-DJK	-DK	d1	d2
A	1.0000							
B	-0.1511	1.0000						
C	0.0782	0.0941	1.0000					
-DJ	0.1991	-0.6955	-0.4348	1.0000				
-DJK	-0.4324	0.1924	-0.0262	-0.6331	1.0000			
-DK	0.0540	0.0233	0.1043	0.4072	-0.8698	1.0000		
d1	0.2397	-0.7212	0.3443	0.5480	-0.4402	0.2657	1.0000	
d2	0.1050	-0.1430	0.1475	-0.1581	0.2747	-0.3326	0.1543	1.0000

Mean value of |C.ij|, i.ne.j = 0.2954
Mean value of C.ij, i.ne.j = -0.0645

Worst fitting lines (obs-calc/error):

442:	-2.2	390:	-1.7	423:	1.5	268:	-1.1
457:	-0.8	455:	0.7	373:	-0.7	407:	0.7
293:	-0.6	425:	0.6	398:	0.6	32:	0.6
182:	-0.6	326:	-0.5	362:	0.5	116:	0.5
175:	-0.5	208:	-0.5	265:	-0.5	364:	0.5
319:	-0.4	296:	0.4	365:	0.4	392:	0.4
354:	0.4	427:	0.4	43:	-0.4	368:	0.3
307:	-0.3	360:	0.3	449:	0.3	372:	0.3
343:	-0.3	99:	0.3	207:	0.3	377:	0.3
272:	-0.3	432:	-0.3	344:	-0.3	366:	0.3
314:	-0.3	350:	0.3	181:	0.3	309:	-0.3
34:	0.3	263:	-0.3	381:	0.3	439:	0.3
387:	0.3	356:	0.3				

SPFIT output reformatted with PIFORM

Heptamer - 7 II

								obs	o-c	error	blends o-c	blends wt	Notes
1:	6	0	6	5	1	5		2018.8362	0.0004	0.025	-0.0010	0.25	
2:	6	1	6	5	0	5		2018.8362	-0.0023	0.025	-0.0010	0.25	
3:	6	0	6	5	0	5		2018.8362	-0.0021	0.025	-0.0010	0.25	
4:	6	1	6	5	1	5		2018.8362	0.0002	0.025	-0.0010	0.25	
5:	6	1	5	5	2	4		2135.7497	0.0017	0.025	-0.0124	0.50	
6:	6	2	5	5	2	4		2135.7497	-0.0265	0.025	-0.0124	0.50	
7:	6	1	5	5	1	4		2136.0344	0.0212	0.025	0.0071	0.50	
8:	6	2	5	5	1	4		2136.0344	-0.0070	0.025	0.0071	0.50	
9:	6	2	4	5	3	3		2249.2964	0.0146	0.025			
10:	6	3	4	5	3	3		2250.5780	0.0000	0.025			
11:	6	2	4	5	2	3		2257.4442	-0.0045	0.025			
12:	6	3	4	5	2	3		2258.7442	-0.0008	0.025			
13:	7	0	7	6	1	6		2345.5582	-0.0011	0.025	-0.0013	0.25	
14:	7	1	7	6	0	6		2345.5582	-0.0014	0.025	-0.0013	0.25	
15:	7	0	7	6	0	6		2345.5582	-0.0014	0.025	-0.0013	0.25	
16:	7	1	7	6	1	6		2345.5582	-0.0012	0.025	-0.0013	0.25	
17:	7	1	6	6	2	5		2462.5296	-0.0042	0.025	-0.0056	0.50	
18:	7	2	6	6	2	5		2462.5296	-0.0069	0.025	-0.0056	0.50	
19:	7	1	6	6	1	5		2462.5689	0.0068	0.025	0.0054	0.50	
20:	7	2	6	6	1	5		2462.5689	0.0040	0.025	0.0054	0.50	
21:	7	2	5	6	3	4		2579.3122	-0.0012	0.025			
22:	7	3	5	6	3	4		2579.5149	0.0345	0.025			
23:	7	2	5	6	2	4		2580.6085	-0.0011	0.025			
24:	7	3	5	6	2	4		2580.7760	-0.0006	0.025			
25:	6	5	2	5	4	1		2595.9318	0.0034	0.025			
26:	8	0	8	7	0	7		2672.2806	-0.0013	0.025	-0.0013	0.25	
27:	8	1	8	7	1	7		2672.2806	-0.0013	0.025	-0.0013	0.25	
28:	8	1	8	7	0	7		2672.2806	-0.0013	0.025	-0.0013	0.25	
29:	8	0	8	7	1	7		2672.2806	-0.0013	0.025	-0.0013	0.25	
30/	7	3	4	6	4	3		2686.2940	0.1353	0.025			
31:	7	4	4	6	3	3		2713.5181	0.0011	0.025			
32:	6	6	1	5	5	0		2716.9813	0.0007	0.025			
33:	6	6	0	5	5	1		2729.0612	0.0006	0.025			
34:	8	2	6	7	3	5		2906.3732	-0.0095	0.025			
35:	8	2	6	7	2	5		2906.5760	0.0262	0.025	0.0168	0.50	
36:	8	3	6	7	2	5		2906.5760	0.0073	0.025	0.0168	0.50	
37:	9	0	9	8	0	8		2999.0018	-0.0016	0.025	-0.0016	0.25	
38:	9	1	9	8	1	8		2999.0018	-0.0016	0.025	-0.0016	0.25	
39:	9	1	9	8	0	8		2999.0018	-0.0016	0.025	-0.0016	0.25	
40:	9	0	9	8	1	8		2999.0018	-0.0016	0.025	-0.0016	0.25	
41:	8	3	5	7	4	4		3022.2839	-0.0013	0.025			
42:	8	4	5	7	4	4		3022.9894	-0.0020	0.025			
43:	8	3	5	7	3	4		3026.8604	-0.0016	0.025			
44:	8	4	5	7	3	4		3027.5674	-0.0008	0.025			
45:	8	4	4	7	5	3		3114.6685	-0.0019	0.025			
46:	9	1	8	8	2	7		3115.9399	-0.0008	0.025	-0.0010	0.25	
47:	9	2	8	8	1	7		3115.9399	-0.0011	0.025	-0.0010	0.25	
48:	9	1	8	8	1	7		3115.9399	-0.0010	0.025	-0.0010	0.25	
49:	9	2	8	8	2	7		3115.9399	-0.0008	0.025	-0.0010	0.25	
50:	8	5	4	7	5	3		3127.5988	-0.0033	0.025			
51:	8	4	4	7	4	3		3165.4011	0.0010	0.025			
52:	7	7	1	6	6	0		3179.2110	-0.0003	0.025			
53:	7	7	0	6	6	1		3185.0026	0.0012	0.025			
54:	9	2	7	8	3	6		3233.0541	0.0087	0.025	-0.0017	0.25	
55:	9	3	7	8	3	6		3233.0541	0.0068	0.025	-0.0017	0.25	
56:	9	2	7	8	2	6		3233.0541	-0.0101	0.025	-0.0017	0.25	
57:	9	3	7	8	2	6		3233.0541	-0.0120	0.025	-0.0017	0.25	
58:	8	5	3	7	5	2		3285.2962	-0.0010	0.025			
59:	10	0	10	9	1	9		3325.7223	-0.0009	0.025	-0.0010	0.25	
60:	10	0	10	9	0	9		3325.7223	-0.0009	0.025	-0.0010	0.25	
61:	10	1	10	9	1	9		3325.7223	-0.0009	0.025	-0.0010	0.25	
62:	10	1	10	9	0	9		3325.7223	-0.0009	0.025	-0.0010	0.25	
63:	9	3	6	8	4	5		3350.4100	-0.0011	0.025			
64:	9	4	6	8	4	5		3350.5018	-0.0020	0.025			

65:	9	3	6	8	3	5	3351.1148	-0.0025	0.025		
66:	9	4	6	8	3	5	3351.2100	0.0000	0.025		
67:	8	6	3	7	5	2	3380.3109	0.0053	0.025		
68:	10	1	9	9	2	8	3442.6477	-0.0009	0.025	-0.0009	0.25
69:	10	2	9	9	1	8	3442.6477	-0.0009	0.025	-0.0009	0.25
70:	10	1	9	9	1	8	3442.6477	-0.0009	0.025	-0.0009	0.25
71:	10	2	9	9	2	8	3442.6477	-0.0009	0.025	-0.0009	0.25
72:	9	4	5	8	5	4	3463.3505	-0.0011	0.025		
73:	9	5	5	8	5	4	3465.7351	-0.0003	0.025		
74:	9	4	5	8	4	4	3476.2823	-0.0010	0.025		
75:	9	5	5	8	4	4	3478.6669	-0.0001	0.025		
76:	9	5	4	8	6	3	3529.2244	-0.0016	0.025		
77:	8	7	2	7	6	1	3550.5384	0.0002	0.025		
78:	10	2	8	9	3	7	3559.6946	0.0000	0.025	-0.0011	0.25
79:	10	3	8	9	2	7	3559.6946	-0.0021	0.025	-0.0011	0.25
80:	10	2	8	9	2	7	3559.6946	-0.0020	0.025	-0.0011	0.25
81:	10	3	8	9	3	7	3559.6946	-0.0002	0.025	-0.0011	0.25
82:	9	6	4	8	6	3	3559.8985	-0.0016	0.025		
83:	8	7	1	7	6	2	3605.3621	-0.0014	0.025		
84:	9	5	4	8	5	3	3624.2353	0.0009	0.025		
85:	8	8	1	7	7	0	3639.8759	0.0002	0.025		
86:	8	8	0	7	7	1	3642.5285	0.0011	0.025		
87:	11	0	11	10	0	10	3652.4393	-0.0018	0.025	-0.0019	0.25
88:	11	1	11	10	1	10	3652.4393	-0.0018	0.025	-0.0019	0.25
89:	11	1	11	10	0	10	3652.4393	-0.0018	0.025	-0.0019	0.25
90:	11	0	11	10	1	10	3652.4393	-0.0018	0.025	-0.0019	0.25
91:	9	6	4	8	5	3	3654.9031	-0.0053	0.025		
92:	9	6	3	8	6	2	3713.6545	-0.0005	0.025		
93:	11	1	10	10	1	9	3769.3567	-0.0014	0.025	-0.0015	0.25
94:	11	2	10	10	2	9	3769.3567	-0.0014	0.025	-0.0015	0.25
95:	11	2	10	10	1	9	3769.3567	-0.0014	0.025	-0.0015	0.25
96:	11	1	10	10	2	9	3769.3567	-0.0014	0.025	-0.0015	0.25
97:	10	4	6	9	5	5	3794.4448	-0.0023	0.025		
98:	10	5	6	9	5	5	3794.8061	-0.0025	0.025		
99:	10	4	6	9	4	5	3796.8296	-0.0013	0.025		
100:	10	5	6	9	4	5	3797.1907	-0.0016	0.025		
101:	9	7	3	8	6	2	3869.3975	0.0012	0.025		
102:	11	2	9	10	3	8	3886.3620	-0.0013	0.025	-0.0015	0.25
103:	11	3	9	10	2	8	3886.3620	-0.0015	0.025	-0.0015	0.25
104:	11	2	9	10	2	8	3886.3620	-0.0015	0.025	-0.0015	0.25
105:	11	3	9	10	3	8	3886.3620	-0.0013	0.025	-0.0015	0.25
106:	10	5	5	9	6	4	3899.9601	-0.0009	0.025		
107:	10	6	5	9	6	4	3906.7479	-0.0019	0.025		
108:	10	5	5	9	5	4	3930.6333	-0.0018	0.025		
109:	10	6	5	9	5	4	3937.4257	0.0017	0.025		
110:	12	0	12	11	0	11	3979.1543	-0.0025	0.025	-0.0025	0.25
111:	12	1	12	11	1	11	3979.1543	-0.0025	0.025	-0.0025	0.25
112:	12	1	12	11	0	11	3979.1543	-0.0025	0.025	-0.0025	0.25
113:	12	0	12	11	1	11	3979.1543	-0.0025	0.025	-0.0025	0.25
114:	9	8	2	8	7	1	4021.7862	0.0021	0.025		
115:	9	8	1	8	7	2	4051.9875	0.0006	0.025		
116:	10	6	4	9	6	3	4079.7353	0.0001	0.025		
117:	9	7	2	8	6	3	4089.1366	-0.0029	0.025		
118:	12	1	11	11	1	10	4096.0659	-0.0019	0.025	-0.0019	0.25
119:	12	2	11	11	2	10	4096.0659	-0.0019	0.025	-0.0019	0.25
120:	12	2	11	11	1	10	4096.0659	-0.0019	0.025	-0.0019	0.25
121:	12	1	11	11	2	10	4096.0659	-0.0019	0.025	-0.0019	0.25
122:	9	9	1	8	8	0	4099.6879	0.0007	0.025		
123:	9	9	0	8	8	1	4100.8643	0.0019	0.025		
124:	11	4	7	10	5	6	4121.4174	0.0009	0.025		
125:	11	5	7	10	5	6	4121.4590	-0.0055	0.025		
126:	11	4	7	10	4	6	4121.7742	-0.0037	0.025		
127:	11	5	7	10	4	6	4121.8195	-0.0064	0.025		
128:	10	7	3	9	7	2	4127.8863	-0.0020	0.025		
129:	10	7	4	9	6	3	4142.3695	0.0015	0.025		
130:	12	2	10	11	2	9	4213.0443	-0.0009	0.025	-0.0009	0.25
131:	12	3	10	11	3	9	4213.0443	-0.0009	0.025	-0.0009	0.25
132:	12	3	10	11	2	9	4213.0443	-0.0009	0.025	-0.0009	0.25
133:	12	2	10	11	3	9	4213.0443	-0.0009	0.025	-0.0009	0.25
134:	11	5	6	10	6	5	4237.8771	-0.0037	0.025		

135:	11	6	6	10	6	5	4239.0626	-0.0044	0.025	
136:	11	5	6	10	5	5	4244.6693	-0.0003	0.025	
137:	11	6	6	10	5	5	4245.8559	0.0000	0.025	
138:	9	6	3	8	5	4	4265.2762	-0.0070	0.025	
139:	13	0	13	12	0	12	4305.8670	-0.0029	0.025	-0.0029 0.25
140:	13	1	13	12	1	12	4305.8670	-0.0029	0.025	-0.0029 0.25
141:	13	1	13	12	0	12	4305.8670	-0.0029	0.025	-0.0029 0.25
142:	13	0	13	12	1	12	4305.8670	-0.0029	0.025	-0.0029 0.25
143:	12	3	9	11	4	8	4330.2061	-0.0007	0.025	-0.0014 0.25
144:	12	4	9	11	3	8	4330.2061	-0.0020	0.025	-0.0014 0.25
145:	12	3	9	11	3	8	4330.2061	-0.0018	0.025	-0.0014 0.25
146:	12	4	9	11	4	8	4330.2061	-0.0008	0.025	-0.0014 0.25
147:	11	7	5	10	7	4	4344.7836	-0.0016	0.025	
148:	10	8	3	9	7	2	4358.6185	-0.0007	0.025	
149:	11	6	5	10	6	4	4390.6044	-0.0005	0.025	
150:	11	8	4	10	8	3	4407.2382	-0.0008	0.025	
151:	11	7	5	10	6	4	4407.4192	0.0011	0.025	
152:	13	1	12	12	1	11	4422.7739	-0.0023	0.025	-0.0023 0.25
153:	13	2	12	12	2	11	4422.7739	-0.0023	0.025	-0.0023 0.25
154:	13	2	12	12	1	11	4422.7739	-0.0023	0.025	-0.0023 0.25
155:	13	1	12	12	2	11	4422.7739	-0.0023	0.025	-0.0023 0.25
156:	12	4	8	11	5	7	4447.8435	0.0295	0.025	0.0027 0.25
157:	12	5	8	11	5	7	4447.8435	0.0237	0.025	0.0027 0.25
158:	12	4	8	11	4	7	4447.8435	-0.0184	0.025	0.0027 0.25
159:	12	5	8	11	4	7	4447.8435	-0.0242	0.025	0.0027 0.25
160:	10	9	2	9	8	1	4488.3920	0.0001	0.025	
161:	10	9	1	9	8	2	4504.0005	0.0007	0.025	
162:	10	8	2	9	7	3	4507.6269	0.0094	0.025	
163:	11	7	4	10	7	3	4525.8409	0.0005	0.025	
164:	11	8	3	10	8	2	4527.7085	-0.0022	0.025	
165:	13	2	11	12	2	10	4539.7321	-0.0019	0.025	-0.0019 0.25
166:	13	2	11	12	3	10	4539.7321	-0.0019	0.025	-0.0019 0.25
167:	13	3	11	12	2	10	4539.7321	-0.0019	0.025	-0.0019 0.25
168:	13	3	11	12	3	10	4539.7321	-0.0019	0.025	-0.0019 0.25
169:	10	10	1	9	9	0	4559.0746	0.0001	0.025	
170:	10	10	0	9	9	1	4559.5832	0.0006	0.025	
171:	12	5	7	11	6	6	4566.0427	-0.0014	0.025	
172:	12	6	7	11	6	6	4566.2180	-0.0038	0.025	
173:	12	5	7	11	5	6	4567.2301	-0.0002	0.025	
174:	12	6	7	11	5	6	4567.4066	-0.0014	0.025	
175:	14	0	14	13	0	13	4632.5781	-0.0021	0.025	-0.0022 0.25
176:	14	1	14	13	1	13	4632.5781	-0.0021	0.025	-0.0022 0.25
177:	14	1	14	13	0	13	4632.5781	-0.0021	0.025	-0.0022 0.25
178:	14	0	14	13	1	13	4632.5781	-0.0021	0.025	-0.0022 0.25
179:	13	3	10	12	4	9	4656.8276	-0.0016	0.025	-0.0017 0.25
180:	13	4	10	12	4	9	4656.8276	-0.0016	0.025	-0.0017 0.25
181:	13	3	10	12	3	9	4656.8276	-0.0017	0.025	-0.0017 0.25
182:	13	4	10	12	3	9	4656.8276	-0.0017	0.025	-0.0017 0.25
183:	12	7	6	11	7	5	4682.7167	0.0051	0.025	
184:	12	6	6	11	6	5	4696.1133	-0.0172	0.025	
185:	12	7	6	11	6	5	4699.5233	-0.0013	0.025	
186:	13	4	9	12	5	8	4774.2509	0.0018	0.025	-0.0014 0.25
187:	13	5	9	12	5	8	4774.2509	0.0011	0.025	-0.0014 0.25
188:	13	4	9	12	4	8	4774.2509	-0.0040	0.025	-0.0014 0.25
189:	13	5	9	12	4	8	4774.2509	-0.0046	0.025	-0.0014 0.25
190:	12	8	5	11	8	4	4778.5272	-0.0019	0.025	
191:	11	9	3	10	8	2	4843.8739	-0.0120	0.025	
192:	14	2	12	13	2	11	4866.4245	-0.0016	0.025	-0.0016 0.25
193:	14	3	12	13	3	11	4866.4245	-0.0016	0.025	-0.0016 0.25
194:	14	3	12	13	2	11	4866.4245	-0.0016	0.025	-0.0016 0.25
195:	14	2	12	13	3	11	4866.4245	-0.0016	0.025	-0.0016 0.25
196:	11	9	2	10	8	3	4936.8967	-0.0015	0.025	
197:	10	6	4	9	5	5	4879.2797	-0.0032	0.025	
198:	11	10	2	10	9	1	4951.6522	-0.0013	0.025	
199:	15	0	15	14	0	14	4959.2858	-0.0016	0.025	-0.0017 0.25
200:	15	1	15	14	1	14	4959.2858	-0.0016	0.025	-0.0017 0.25
201:	15	1	15	14	0	14	4959.2858	-0.0016	0.025	-0.0017 0.25
202:	15	0	15	14	1	14	4959.2858	-0.0016	0.025	-0.0017 0.25
203:	11	10	1	10	9	2	4959.3435	0.0008	0.025	
204:	14	3	11	13	3	10	4983.4743	-0.0009	0.025	-0.0009 0.25

205:	14	4	11	13	4	10	4983.4743	-0.0009	0.025	-0.0009	0.25
206:	14	4	11	13	3	10	4983.4743	-0.0009	0.025	-0.0009	0.25
207:	14	3	11	13	4	10	4983.4743	-0.0009	0.025	-0.0009	0.25
208:	13	6	7	12	7	6	5010.7332	-0.0001	0.025		
209:	13	7	7	12	7	6	5011.3084	0.0028	0.025		
210:	13	6	7	12	6	6	5014.1241	-0.0033	0.025		
211:	13	7	7	12	6	6	5014.6958	-0.0039	0.025		
212:	11	11	1	10	10	0	5018.2620	0.0022	0.025		
213:	15	1	14	14	1	13	5076.1849	-0.0019	0.025	-0.0019	0.25
214:	15	2	14	14	2	13	5076.1849	-0.0019	0.025	-0.0019	0.25
215:	15	2	14	14	1	13	5076.1849	-0.0019	0.025	-0.0019	0.25
216:	15	1	14	14	2	13	5076.1849	-0.0019	0.025	-0.0019	0.25
217:	14	4	10	13	5	9	5100.7627	-0.0009	0.025	-0.0013	0.25
218:	14	5	10	13	4	9	5100.7627	-0.0016	0.025	-0.0013	0.25
219:	14	4	10	13	4	9	5100.7627	-0.0015	0.025	-0.0013	0.25
220:	14	5	10	13	5	9	5100.7627	-0.0010	0.025	-0.0013	0.25
221:	13	7	6	12	8	5	5116.1645	0.0012	0.025		
222:	13	8	6	12	8	5	5124.8082	-0.0037	0.025		
223:	12	9	4	11	8	3	5137.9158	0.0032	0.025		
224:	13	8	6	12	7	5	5161.6046	0.0037	0.025		
225:	15	2	13	14	2	12	5193.1180	-0.0011	0.025	-0.0011	0.25
226:	15	3	13	14	3	12	5193.1180	-0.0011	0.025	-0.0011	0.25
227:	15	3	13	14	2	12	5193.1180	-0.0011	0.025	-0.0011	0.25
228:	15	2	13	14	3	12	5193.1180	-0.0011	0.025	-0.0011	0.25
229:	13	9	5	12	9	4	5206.8664	-0.0020	0.025		
230:	16	0	16	15	0	15	5285.9895	-0.0020	0.025	-0.0020	0.25
231:	16	1	16	15	1	15	5285.9895	-0.0020	0.025	-0.0020	0.25
232:	16	1	16	15	0	15	5285.9895	-0.0020	0.025	-0.0020	0.25
233:	16	0	16	15	1	15	5285.9895	-0.0020	0.025	-0.0020	0.25
234:	15	3	12	14	3	11	5310.1344	-0.0005	0.025	-0.0005	0.25
235:	15	4	12	14	4	11	5310.1344	-0.0005	0.025	-0.0005	0.25
236:	15	4	12	14	3	11	5310.1344	-0.0005	0.025	-0.0005	0.25
237:	15	3	12	14	4	11	5310.1344	-0.0005	0.025	-0.0005	0.25
238:	13	8	5	12	8	4	5314.7081	0.0020	0.025		
239:	12	10	3	11	9	2	5322.5882	0.0018	0.025		
240:	14	6	8	13	7	7	5337.3122	0.0010	0.025		
241:	14	7	8	13	7	7	5337.4066	0.0104	0.025		
242:	14	6	8	13	6	7	5337.8857	0.0022	0.025		
243:	14	7	8	13	6	7	5337.9672	-0.0012	0.025		
244:	12	10	2	11	9	3	5376.4347	-0.0005	0.025		
245:	16	1	15	15	1	14	5402.8873	-0.0006	0.025	-0.0007	0.25
246:	16	2	15	15	2	14	5402.8873	-0.0006	0.025	-0.0007	0.25
247:	16	2	15	15	1	14	5402.8873	-0.0006	0.025	-0.0007	0.25
248:	16	1	15	15	2	14	5402.8873	-0.0006	0.025	-0.0007	0.25
249:	12	11	2	11	10	1	5412.8918	0.0003	0.025		
250:	12	11	1	11	10	2	5416.5459	0.0007	0.025		
251:	15	4	11	14	4	10	5427.3330	0.0003	0.025	0.0004	0.25
252:	15	5	11	14	4	10	5427.3330	0.0003	0.025	0.0004	0.25
253:	15	5	11	14	5	10	5427.3330	0.0004	0.025	0.0004	0.25
254:	15	4	11	14	5	10	5427.3330	0.0004	0.025	0.0004	0.25
255:	12	9	3	11	8	4	5445.2436	0.0012	0.025		
256:	14	8	7	13	8	6	5456.4518	-0.0035	0.025		
257:	14	7	7	13	7	6	5463.4606	-0.0010	0.025		
258:	14	8	7	13	7	6	5465.1035	-0.0004	0.025		
259:	11	6	5	10	5	6	5475.0801	0.0008	0.025		
260:	12	12	1	11	11	0	5477.3521	0.0021	0.025		
261:	12	12	0	11	11	1	5477.4423	0.0021	0.025		
262:	16	2	14	15	2	13	5519.8113	-0.0001	0.025	-0.0002	0.25
263:	16	3	14	15	3	13	5519.8113	-0.0001	0.025	-0.0002	0.25
264:	16	3	14	15	2	13	5519.8113	-0.0001	0.025	-0.0002	0.25
265:	16	2	14	15	3	13	5519.8113	-0.0001	0.025	-0.0002	0.25
266:	15	5	10	14	6	9	5544.9123	0.0019	0.025	0.0003	0.25
267:	15	6	10	14	6	9	5544.9123	0.0015	0.025	0.0003	0.25
268:	15	5	10	14	5	9	5544.9123	-0.0010	0.025	0.0003	0.25
269:	15	6	10	14	5	9	5544.9123	-0.0013	0.025	0.0003	0.25
270:	14	9	6	13	9	5	5564.1433	-0.0022	0.025		
271:	14	8	6	13	8	5	5615.9652	0.0043	0.025		
272:	16	3	13	15	3	12	5636.8024	0.0001	0.025	0.0001	0.25
273:	16	4	13	15	4	12	5636.8024	0.0001	0.025	0.0001	0.25
274:	16	4	13	15	3	12	5636.8024	0.0001	0.025	0.0001	0.25

275:	16	3	13	15	4	12	5636.8024	0.0001	0.025	0.0001	0.25
276:	17	1	16	16	1	15	5729.5842	-0.0017	0.025	-0.0018	0.25
277:	17	2	16	16	2	15	5729.5842	-0.0017	0.025	-0.0018	0.25
278:	17	2	16	16	1	15	5729.5842	-0.0017	0.025	-0.0018	0.25
279:	17	1	16	16	2	15	5729.5842	-0.0017	0.025	-0.0018	0.25
280:	16	4	12	15	4	11	5753.9347	-0.0004	0.025	-0.0005	0.25
281:	16	5	12	15	5	11	5753.9347	-0.0004	0.025	-0.0005	0.25
282:	16	5	12	15	4	11	5753.9347	-0.0004	0.025	-0.0005	0.25
283:	16	4	12	15	5	11	5753.9347	-0.0004	0.025	-0.0005	0.25
284:	15	7	8	14	8	7	5782.6347	0.0020	0.025		
285:	15	8	8	14	8	7	5782.8993	-0.0032	0.025		
286:	15	7	8	14	7	7	5784.2711	-0.0037	0.025		
287:	15	8	8	14	7	7	5784.5449	0.0000	0.025		
288:	13	11	3	12	10	2	5794.5464	0.0004	0.025		
289:	13	11	2	12	10	3	5823.8486	0.0020	0.025		
290:	17	2	15	16	2	14	5846.5022	0.0000	0.025	-0.0001	0.25
291:	17	3	15	16	3	14	5846.5022	0.0000	0.025	-0.0001	0.25
292:	17	3	15	16	2	14	5846.5022	0.0000	0.025	-0.0001	0.25
293:	17	2	15	16	3	14	5846.5022	0.0000	0.025	-0.0001	0.25
294:	13	10	3	12	9	4	5851.5865	0.0023	0.025		
295:	16	5	11	15	6	10	5871.3545	0.0008	0.025	0.0006	0.25
296:	16	6	11	15	5	10	5871.3545	0.0004	0.025	0.0006	0.25
297:	16	5	11	15	5	10	5871.3545	0.0004	0.025	0.0006	0.25
298:	16	6	11	15	6	10	5871.3545	0.0007	0.025	0.0006	0.25
299:	13	12	1	12	11	2	5874.7146	0.0030	0.025		
300:	18	0	18	17	0	17	5939.3873	-0.0013	0.025	-0.0014	0.25
301:	18	1	18	17	1	17	5939.3873	-0.0013	0.025	-0.0014	0.25
302:	18	1	18	17	0	17	5939.3873	-0.0013	0.025	-0.0014	0.25
303:	18	0	18	17	1	17	5939.3873	-0.0013	0.025	-0.0014	0.25
304:	17	3	14	16	3	13	5963.4738	0.0001	0.025	0.0002	0.25
305:	17	4	14	16	4	13	5963.4738	0.0001	0.025	0.0002	0.25
306:	17	4	14	16	3	13	5963.4738	0.0001	0.025	0.0002	0.25
307:	17	3	14	16	4	13	5963.4738	0.0001	0.025	0.0002	0.25
308:	16	6	10	15	7	9	5989.3475	0.0064	0.025	0.0000	0.25
309:	16	7	10	15	7	9	5989.3475	0.0050	0.025	0.0000	0.25
310:	16	6	10	15	6	9	5989.3475	-0.0050	0.025	0.0000	0.25
311:	16	7	10	15	6	9	5989.3475	-0.0064	0.025	0.0000	0.25
312:	18	1	17	17	1	16	6056.2793	-0.0010	0.025	-0.0011	0.25
313:	18	1	17	17	2	16	6056.2793	-0.0010	0.025	-0.0011	0.25
314:	18	2	17	17	1	16	6056.2793	-0.0010	0.025	-0.0011	0.25
315:	18	2	17	17	2	16	6056.2793	-0.0010	0.025	-0.0011	0.25
316:	17	4	13	16	4	12	6080.5595	0.0007	0.025	0.0008	0.25
317:	17	4	13	16	5	12	6080.5595	0.0007	0.025	0.0008	0.25
318:	17	5	13	16	4	12	6080.5595	0.0007	0.025	0.0008	0.25
319:	17	5	13	16	5	12	6080.5595	0.0007	0.025	0.0008	0.25
320:	15	9	6	14	9	5	6083.1945	0.0043	0.025		
321:	17	5	12	16	5	11	6197.8670	0.0024	0.025	0.0024	0.25
322:	17	5	12	16	6	11	6197.8670	0.0024	0.025	0.0024	0.25
323:	17	6	12	16	6	11	6197.8670	0.0024	0.025	0.0024	0.25
324:	17	6	12	16	5	11	6197.8670	0.0024	0.025	0.0024	0.25
325:	16	8	8	15	9	7	6228.0575	0.0027	0.025		
326:	16	9	8	15	9	7	6228.7838	-0.0472	0.025		
327:	16	8	8	15	8	7	6232.2890	-0.0335	0.025		
328:	16	9	8	15	8	7	6233.0977	-0.0009	0.025		
329:	14	12	3	13	11	2	6261.2656	0.0011	0.025		
330:	19	0	19	18	0	18	6266.0807	-0.0006	0.025	-0.0007	0.25
331:	19	1	19	18	1	18	6266.0807	-0.0006	0.025	-0.0007	0.25
332:	19	1	19	18	0	18	6266.0807	-0.0006	0.025	-0.0007	0.25
333:	19	0	19	18	1	18	6266.0807	-0.0006	0.025	-0.0007	0.25
334:	14	11	3	13	10	4	6270.6680	-0.0026	0.025		
335:	14	12	2	13	11	3	6276.4587	0.0023	0.025		
336:	18	3	15	17	3	14	6290.1469	0.0003	0.025	0.0003	0.25
337:	18	4	15	17	4	14	6290.1469	0.0003	0.025	0.0003	0.25
338:	18	4	15	17	3	14	6290.1469	0.0003	0.025	0.0003	0.25
339:	18	3	15	17	4	14	6290.1469	0.0003	0.025	0.0003	0.25
340:	14	13	2	13	12	1	6332.5865	0.0016	0.025		
341:	14	13	1	13	12	2	6333.3511	0.0037	0.025		
342:	19	1	18	18	1	17	6382.9706	-0.0004	0.025	-0.0004	0.25
343:	19	2	18	18	2	17	6382.9706	-0.0004	0.025	-0.0004	0.25
344:	19	2	18	18	1	17	6382.9706	-0.0004	0.025	-0.0004	0.25

345:	19	1	18	18	2	17	6382.9706	-0.0004	0.025	-0.0004	0.25	
346:	14	14	1	13	13	0	6395.4218	0.0088	0.025	0.0012	0.50	
347:	14	14	0	13	13	1	6395.4218	-0.0063	0.025	0.0012	0.50	
348:	14	14	0	13	13	0	6395.4216	0.0042	0.025	0.0010	0.50	uc
349:	14	14	1	13	13	1	6395.4216	-0.0021	0.025	0.0010	0.50	uc
350:	18	4	14	17	4	13	6407.1957	0.0005	0.025	0.0005	0.25	
351:	18	5	14	17	5	13	6407.1957	0.0005	0.025	0.0005	0.25	
352:	18	5	14	17	4	13	6407.1957	0.0005	0.025	0.0005	0.25	
353:	18	4	14	17	5	13	6407.1957	0.0005	0.025	0.0005	0.25	
354:	16	11	6	15	11	5	6429.3058	-0.0303	0.025			
355:	18	5	13	17	5	12	6524.4206	0.0019	0.025	0.0020	0.25	
356:	18	5	13	17	6	12	6524.4206	0.0019	0.025	0.0020	0.25	
357:	18	6	13	17	5	12	6524.4206	0.0019	0.025	0.0020	0.25	
358:	18	6	13	17	6	12	6524.4206	0.0019	0.025	0.0020	0.25	
359:	16	10	6	15	10	5	6549.0699	0.0017	0.025			
360:	20	0	20	19	0	19	6592.7706	0.0006	0.025	0.0006	0.25	
361:	20	1	20	19	1	19	6592.7706	0.0006	0.025	0.0006	0.25	
362:	20	1	20	19	0	19	6592.7706	0.0006	0.025	0.0006	0.25	
363:	20	0	20	19	1	19	6592.7706	0.0006	0.025	0.0006	0.25	
364:	19	3	16	18	3	15	6616.8206	0.0013	0.025	0.0013	0.25	
365:	19	4	16	18	4	15	6616.8206	0.0013	0.025	0.0013	0.25	
366:	19	4	16	18	3	15	6616.8206	0.0013	0.025	0.0013	0.25	
367:	19	3	16	18	4	15	6616.8206	0.0013	0.025	0.0013	0.25	
368:	18	6	12	17	7	11	6641.9667	0.0010	0.025	0.0009	0.25	
369:	18	7	12	17	6	11	6641.9667	0.0008	0.025	0.0009	0.25	
370:	18	6	12	17	6	11	6641.9667	0.0008	0.025	0.0009	0.25	
371:	18	7	12	17	7	11	6641.9667	0.0010	0.025	0.0009	0.25	
372:	17	10	8	16	10	7	6674.9303	0.0112	0.025			
373:	15	12	3	14	11	4	6702.4727	0.0027	0.025			
374:	20	1	19	19	1	18	6709.6573	-0.0002	0.025	-0.0002	0.25	
375:	20	2	19	19	2	18	6709.6573	-0.0002	0.025	-0.0002	0.25	
376:	20	2	19	19	1	18	6709.6573	-0.0002	0.025	-0.0002	0.25	
377:	20	1	19	19	2	18	6709.6573	-0.0002	0.025	-0.0002	0.25	
378:	15	13	3	14	12	2	6724.5662	-0.0005	0.025			
379:	15	13	2	14	12	3	6732.1593	0.0048	0.025			
380:	19	4	15	18	4	14	6733.8400	0.0007	0.025	0.0007	0.25	
381:	19	4	15	18	5	14	6733.8400	0.0007	0.025	0.0007	0.25	
382:	19	5	15	18	4	14	6733.8400	0.0007	0.025	0.0007	0.25	
383:	19	5	15	18	5	14	6733.8400	0.0007	0.025	0.0007	0.25	
384:	18	7	11	17	8	10	6760.1197	0.0045	0.025	0.0015	0.25	
385:	18	8	11	17	8	10	6760.1197	0.0038	0.025	0.0015	0.25	
386:	18	7	11	17	7	10	6760.1197	-0.0008	0.025	0.0015	0.25	
387:	18	8	11	17	7	10	6760.1197	-0.0015	0.025	0.0015	0.25	
388:	17	10	7	16	11	6	6762.8570	0.0045	0.025			
389:	15	14	2	14	13	1	6791.8634	0.0042	0.025			
390:	15	14	1	14	13	2	6792.1938	-0.0034	0.025			
391:	20	2	18	19	2	17	6826.5592	0.0012	0.025	0.0013	0.25	
392:	20	3	18	19	3	17	6826.5592	0.0012	0.025	0.0013	0.25	
393:	20	3	18	19	2	17	6826.5592	0.0012	0.025	0.0013	0.25	
394:	20	2	18	19	3	17	6826.5592	0.0012	0.025	0.0013	0.25	
395:	15	15	1	14	14	0	6854.4206	0.0041	0.025	0.0011	0.50	
396:	15	15	0	14	14	1	6854.4206	-0.0019	0.025	0.0011	0.50	
397:	15	15	0	14	14	0	6854.4204	0.0021	0.025	0.0009	0.50	uc
398:	15	15	1	14	14	1	6854.4204	-0.0004	0.025	0.0009	0.50	uc
399:	20	3	17	19	3	16	6943.4910	0.0002	0.025	0.0003	0.25	
400:	20	4	17	19	4	16	6943.4910	0.0002	0.025	0.0003	0.25	
401:	20	4	17	19	3	16	6943.4910	0.0002	0.025	0.0003	0.25	
402:	20	3	17	19	4	16	6943.4910	0.0002	0.025	0.0003	0.25	
403:	19	6	13	18	6	12	6968.4199	0.0038	0.025	0.0039	0.25	
404:	19	6	13	18	7	12	6968.4199	0.0038	0.025	0.0039	0.25	
405:	19	7	13	18	6	12	6968.4199	0.0038	0.025	0.0039	0.25	
406:	19	7	13	18	7	12	6968.4199	0.0038	0.025	0.0039	0.25	
407:	18	9	9	17	9	8	7002.1242	0.0064	0.025			
408:	18	10	9	17	9	8	7002.4844	0.0062	0.025			
409:	17	11	6	16	11	5	7006.2995	0.0119	0.025			
410:	20	4	16	19	4	15	7060.4898	0.0021	0.025	0.0021	0.25	
411:	20	5	16	19	5	15	7060.4898	0.0021	0.025	0.0021	0.25	
412:	20	5	16	19	4	15	7060.4898	0.0021	0.025	0.0021	0.25	
413:	20	4	16	19	5	15	7060.4898	0.0021	0.025	0.0021	0.25	
414:	19	7	12	18	8	11	7086.2932	0.0059	0.025	0.0056	0.25	

415:	19	8	12	18	7	11	7086.2932	0.0052	0.025	0.0056	0.25	
416:	19	7	12	18	7	11	7086.2932	0.0052	0.025	0.0056	0.25	
417:	19	8	12	18	8	11	7086.2932	0.0058	0.025	0.0056	0.25	
418:	16	13	4	15	12	3	7097.5752	0.0013	0.025			
419:	18	10	8	17	11	7	7115.6421	0.0051	0.025			
420:	16	13	3	15	12	4	7144.5933	0.0032	0.025			
421:	16	14	3	15	13	2	7185.8695	-0.0015	0.025			
422:	16	14	2	15	13	3	7189.5499	-0.0003	0.025			
423:	16	12	4	15	11	5	7198.4618	0.0069	0.025			
424:	19	8	11	18	9	10	7205.0065	0.0166	0.025	0.0062	0.25	
425:	19	9	11	18	9	10	7205.0065	0.0141	0.025	0.0062	0.25	
426:	19	8	11	18	8	10	7205.0065	-0.0017	0.025	0.0062	0.25	
427:	19	9	11	18	8	10	7205.0065	-0.0042	0.025	0.0062	0.25	
428:	16	15	2	15	14	1	7250.9952	0.0062	0.025			
429:	16	15	1	15	14	2	7251.1349	-0.0015	0.025			
430:	20	6	14	19	7	13	7294.9241	0.0061	0.025	0.0061	0.25	
431:	20	7	14	19	6	13	7294.9241	0.0060	0.025	0.0061	0.25	
432:	20	6	14	19	6	13	7294.9241	0.0060	0.025	0.0061	0.25	
433:	20	7	14	19	7	13	7294.9241	0.0061	0.025	0.0061	0.25	
434:	16	16	1	15	15	0	7313.4151	0.0070	0.025	0.0058	0.50	
435:	16	16	0	15	15	1	7313.4151	0.0045	0.025	0.0058	0.50	
436:	17	15	3	16	14	2	7646.0781	-0.0011	0.025			
437:	17	15	2	16	14	3	7647.8226	0.0019	0.025			
438:	17	17	1	16	16	0	7772.3827	-0.0065	0.025	-0.0070	0.50	
439:	17	17	0	16	16	1	7772.3827	-0.0075	0.025	-0.0070	0.50	
440:	17	17	1	16	16	1	7772.3825	-0.0074	0.025	-0.0072	0.50	uc
441:	17	17	0	16	16	0	7772.3825	-0.0069	0.025	-0.0072	0.50	uc
442:	15	5	10	14	3	11	7866.3448	-0.0258	0.025	-0.0260	0.25	
443:	15	6	10	14	4	11	7866.3448	-0.0261	0.025	-0.0260	0.25	
444:	15	6	10	14	3	11	7866.3448	-0.0261	0.025	-0.0260	0.25	
445:	15	5	10	14	4	11	7866.3448	-0.0258	0.025	-0.0260	0.25	
446:	5	5	0	4	4	0	2260.4634	0.0021	0.025			uc-lines
447:	5	5	1	4	4	1	2267.8169	-0.0012	0.025			
448:	6	4	2	5	3	2	2626.0601	0.0083	0.025			
449:	6	5	1	5	4	1	2652.5989	0.0040	0.025			
450:	6	5	2	5	4	2	2678.8178	0.0007	0.025			
451:	6	6	0	5	5	0	2720.9328	-0.0050	0.025			
452:	6	6	1	5	5	1	2725.0950	-0.0081	0.025			
453:	7	5	2	6	4	2	3065.1134	0.0024	0.025			
454:	7	4	3	6	3	3	3075.9602	0.0026	0.025			
455:	7	3	4	6	2	4	3096.3579	0.0010	0.025			
456:	7	4	4	6	3	4	3099.6346	-0.0027	0.025			
457:	7	2	5	6	1	5	3101.9912	0.0012	0.025			
458:	7	3	5	6	2	5	3102.1222	-0.0065	0.025			
459:	7	5	3	6	4	3	3103.9063	0.0005	0.025			
460:	7	6	1	6	5	1	3109.5835	0.0008	0.025			
461:	7	6	2	6	5	2	3131.2157	0.0011	0.025			
462:	7	7	0	6	6	0	3181.0454	0.0013	0.025			
463:	7	7	1	6	6	1	3183.1674	-0.0013	0.025			
464:	8	5	3	7	4	3	3505.8373	-0.0007	0.025			
465:	8	6	2	7	5	2	3509.4185	-0.0005	0.025			
466:	8	4	4	7	3	4	3532.4168	-0.0007	0.025			
467:	8	5	4	7	4	4	3540.7713	-0.0010	0.025			
468:	8	3	5	7	2	5	3542.6089	-0.0003	0.025			
469:	8	4	5	7	3	5	3543.1482	-0.0002	0.025			
470:	8	2	6	7	1	6	3545.9832	0.0056	0.025	-0.0024	0.50	
471:	8	3	6	7	2	6	3545.9832	-0.0105	0.025	-0.0024	0.50	
472:	8	6	3	7	5	3	3550.1171	0.0002	0.025			
473:	8	7	1	7	6	1	3570.3311	0.0021	0.025			
474:	8	8	0	7	7	0	3640.6973	0.0026	0.025			
475:	8	8	1	7	7	1	3641.7064	-0.0020	0.025			
476:	9	6	3	8	5	3	3937.7732	-0.0036	0.025			
477:	9	7	2	8	6	2	3960.0257	-0.0004	0.025			
478:	9	5	4	8	4	4	3964.6725	0.0001	0.025			
479:	9	6	4	8	5	4	3982.4120	-0.0028	0.025			
480:	9	8	1	8	7	1	4032.1945	-0.0015	0.025			
481:	9	8	2	8	7	2	4041.5759	0.0009	0.025			
482:	9	9	0	8	8	0	4100.0471	0.0036	0.025			
483:	9	9	1	8	8	1	4100.5034	-0.0026	0.025			
484:	10	7	3	9	6	3	4374.2582	-0.0012	0.025			

485:	10	6	4	9	5	4	4393.2783	0.0006	0.025	
486:	10	8	2	9	7	2	4416.9556	-0.0319	0.025	
487:	10	5	5	9	4	5	4419.0223	-0.0018	0.025	
488:	10	6	5	9	5	5	4423.4327	0.0035	0.025	
489:	10	7	4	9	6	4	4425.2376	0.0012	0.025	
490:	10	4	6	9	3	6	4427.5567	0.0042	0.025	
491:	10	5	6	9	4	6	4427.8383	0.0171	0.025	
492:	10	3	7	9	2	7	4431.2899	0.0047	0.025	0.0002 0.50
493:	10	4	7	9	3	7	4431.2899	-0.0042	0.025	0.0002 0.50
494:	10	2	8	9	1	8	4433.5615	0.0038	0.025	0.0037 0.50
495:	10	3	8	9	2	8	4433.5615	0.0036	0.025	0.0037 0.50
496:	10	8	3	9	7	3	4449.2364	-0.0127	0.025	
497:	10	9	2	9	8	2	4498.8018	-0.0019	0.025	
498:	10	10	0	9	9	0	4559.2313	0.0050	0.025	
499:	10	10	1	9	9	1	4559.4347	0.0040	0.025	
500:	11	8	3	10	7	3	4816.8089	-0.0008	0.025	
501:	11	6	5	10	5	5	4853.2449	-0.0026	0.025	
502:	11	7	5	10	6	5	4863.2755	0.0036	0.025	
503:	11	5	6	10	4	6	4866.8644	0.0014	0.025	
504:	11	8	4	10	7	4	4869.8537	-0.0076	0.025	
505:	11	3	8	10	2	8	4875.2241	0.0021	0.025	0.0016 0.50
506:	11	4	8	10	3	8	4875.2241	0.0011	0.025	0.0016 0.50
507:	11	2	9	10	1	9	4877.2760	0.0033	0.025	0.0033 0.50
508:	11	3	9	10	2	9	4877.2760	0.0033	0.025	0.0033 0.50
509:	11	9	2	10	8	2	4878.5326	0.0026	0.025	
510:	11	9	3	10	8	3	4902.2542	0.0000	0.025	
511:	11	10	1	10	9	1	4954.1561	0.0094	0.025	
512:	11	10	2	10	9	2	4956.8507	0.0011	0.025	
513:	12	8	4	11	7	4	5249.3488	-0.0081	0.025	
514:	12	9	3	11	8	3	5266.4047	0.0021	0.025	
515:	12	7	5	11	6	5	5283.6308	0.0013	0.025	
516:	12	8	5	11	7	5	5303.6053	0.0000	0.025	
517:	12	6	6	11	5	6	5304.7106	0.0021	0.025	
518:	12	4	8	11	3	8	5316.3882	0.0018	0.025	-0.0004 0.50
519:	12	5	8	11	4	8	5316.3882	-0.0027	0.025	-0.0004 0.50
520:	12	9	4	11	8	4	5316.7478	-0.0046	0.025	
521:	12	2	10	11	1	10	5320.9577	-0.0019	0.025	-0.0019 0.50
522:	12	3	10	11	2	10	5320.9577	-0.0019	0.025	-0.0019 0.50
523:	12	10	2	11	9	2	5341.7855	-0.0056	0.025	
524:	12	10	3	11	9	3	5357.2223	-0.0081	0.025	
525:	12	11	1	11	10	1	5414.0537	0.0016	0.025	
526:	12	11	2	11	10	2	5415.3884	0.0038	0.025	
527:	13	9	4	12	8	4	5683.2017	-0.0117	0.025	
528:	13	8	5	12	7	5	5710.1944	0.0011	0.025	
529:	13	7	6	12	6	6	5740.4519	0.0006	0.025	
530:	13	9	5	12	8	5	5745.0963	0.0046	0.025	
531:	13	6	7	12	5	7	5751.6033	-0.0021	0.025	
532:	13	7	7	12	6	7	5752.0005	0.0004	0.025	
533:	13	5	8	12	4	8	5756.9950	0.0061	0.025	-0.0029 0.50
534:	13	6	8	12	5	8	5756.9950	-0.0119	0.025	-0.0029 0.50
535:	13	3	10	12	2	10	5762.8464	-0.0041	0.025	
536:	13	10	4	12	9	4	5766.1507	0.0098	0.025	
537:	13	11	2	12	10	2	5804.6366	-0.0052	0.025	
538:	13	11	3	12	10	3	5813.7501	-0.0006	0.025	
539:	13	12	1	12	11	1	5873.5559	0.0049	0.025	
540:	13	12	2	12	11	2	5874.1816	-0.0025	0.025	
541:	13	13	0	12	12	0	5936.4051	0.0003	0.025	-0.0074 0.50
542:	13	13	1	12	12	1	5936.4051	-0.0152	0.025	-0.0074 0.50
543:	14	10	4	13	9	4	6123.7692	0.0042	0.025	
544:	14	9	5	13	8	5	6134.8485	0.0076	0.025	
545:	14	9	6	13	8	6	6184.4200	-0.0052	0.025	
546:	14	11	3	13	10	3	6185.2294	0.0019	0.025	
547:	14	10	5	13	9	5	6188.3726	-0.0028	0.025	
548:	14	4	10	13	3	10	6204.3982	0.0301	0.025	0.0301 0.50
549:	14	5	10	13	4	10	6204.3982	0.0300	0.025	0.0301 0.50
550:	14	3	11	13	2	11	6206.5629	-0.0288	0.025	-0.0289 0.50
551:	14	4	11	13	3	11	6206.5629	-0.0288	0.025	-0.0289 0.50
552:	14	2	12	13	1	12	6208.2839	0.0080	0.025	0.0080 0.50
553:	14	3	12	13	2	12	6208.2839	0.0080	0.025	0.0080 0.50
554:	14	1	13	13	0	13	6209.5954	0.0089	0.025	0.0089 0.50

```
 555: 14  2 13    13  1 13                    6209.5954   0.0089  0.025   0.0089 0.50
 556: 14 11  4    13 10  4                    6218.0084   0.0061  0.025
 557: 14 12  2    13 11  2                    6266.3598  -0.0006  0.025
 558: 14 12  3    13 11  3                    6271.3665   0.0061  0.025
 559: 14 13  1    13 12  1                    6332.8148  -0.0050  0.025
 560: 14 13  2    13 12  2                    6333.1110  -0.0013  0.025
 561: 15  9  7    14  8  7                    6629.1002   0.0164  0.025
 562: 15  7  8    14  6  8                    6636.1776   0.0006  0.025
 563: 15  8  8    14  7  8                    6636.3695   0.0076  0.025
 564: 15  6  9    14  5  9                    6641.7082   0.0049  0.025   0.0007 0.50
 565: 15  7  9    14  6  9                    6641.7082  -0.0036  0.025   0.0007 0.50
 566: 15  5 10    14  4 10                    6645.4767  -0.0011  0.025  -0.0013 0.50
 567: 15  6 10    14  5 10                    6645.4767  -0.0014  0.025  -0.0013 0.50
 568: 15  4 11    14  3 11                    6648.2274   0.0019  0.025   0.0019 0.50
 569: 15  5 11    14  4 11                    6648.2274   0.0019  0.025   0.0019 0.50
 570: 15 12  3    14 11  3                    6649.7984  -0.0031  0.025
 571: 15 13  3    14 12  3                    6729.6571  -0.0056  0.025
-------------------------------------------------------------------------------

PARAMETERS IN FIT:

       10000            A  /MHz          229.5257(3)                          1
       20000            B  /MHz          215.0008(3)                          2
       30000            C  /MHz          163.3655(2)                          3
         200           DJ  /kHz            0.0084(8)                          4
        1100          DJK  /kHz            0.068(4)                           5
        2000           DK  /kHz           -0.055(4)                           6
       40100           d1  /kHz           -0.0028(3)                          7
       50000           d2  /kHz           -0.0031(2)                          8

 MICROWAVE AVG =        0.000153 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.009707 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.38828         0.38828

  distinct frequency lines in fit:   348
       distinct parameters of fit:     8

 for standard errors previous errors are multiplied by:   0.392821

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

       10000            A  /MHz          229.5257(1)                          1
       20000            B  /MHz          215.0008(1)                          2
       30000            C  /MHz          163.3655(1)                          3
         200           DJ  /kHz            0.0084(3)                          4
        1100          DJK  /kHz            0.068(1)                           5
        2000           DK  /kHz           -0.055(1)                           6
       40100           d1  /kHz           -0.0028(1)                          7
       50000           d2  /kHz           -0.00318(8)                         8

 CORRELATION COEFFICIENTS, C.ij:

           A        B        C       -DJ      -DJK     -DK      d1       d2

A           1.0000
B          -0.2947   1.0000
C          -0.1721   0.1226   1.0000
-DJ         0.4883  -0.7297  -0.3860   1.0000
-DJK       -0.5893   0.4463   0.1460  -0.8613   1.0000
-DK         0.4190  -0.3126  -0.0575   0.7486  -0.9621   1.0000
d1          0.2851  -0.7901   0.2251   0.7082  -0.5885   0.4965   1.0000
d2         -0.2451  -0.0791   0.2140  -0.3525   0.5637  -0.6087  -0.0006   1.0000

 Mean value of |C.ij|, i.ne.j =   0.4248
 Mean value of  C.ij,  i.ne.j =  -0.0774


 Worst fitting lines (obs-calc/error):

    30:    5.4        326:   -1.9         22:    1.4        327:   -1.3
```

486:	-1.3	354:	-1.2	548:	1.2	550:	-1.2
442:	-1.0	184:	-0.7	491:	0.7	35:	0.7
561:	0.7	9:	0.6	496:	-0.5	5:	-0.5
191:	-0.5	409:	0.5	527:	-0.5	372:	0.4
241:	0.4	536:	0.4	34:	-0.4	162:	0.4
511:	0.4	554:	0.4	448:	0.3	513:	-0.3
452:	-0.3	524:	-0.3	552:	0.3	504:	-0.3
544:	0.3	563:	0.3	541:	-0.3	440:	-0.3
7:	0.3	438:	-0.3	138:	-0.3	423:	0.3
458:	-0.3	127:	-0.3	407:	0.3	428:	0.2
408:	0.2	424:	0.2	430:	0.2	556:	0.2
558:	0.2	434:	0.2				

/ SPFIT output reformatted with PIFORM