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Electronic Supplementary Information for:

Solvent-assisted synthesis of shape-persistent chiral polyaza gigantocycle characterized by a very large internal cavity and extraordinarily high amplitude of the ECD exciton couplet

Mikołaj Zgorzelak, Jakub Grajewski, Jacek Gawronski, and Marcin Kwit

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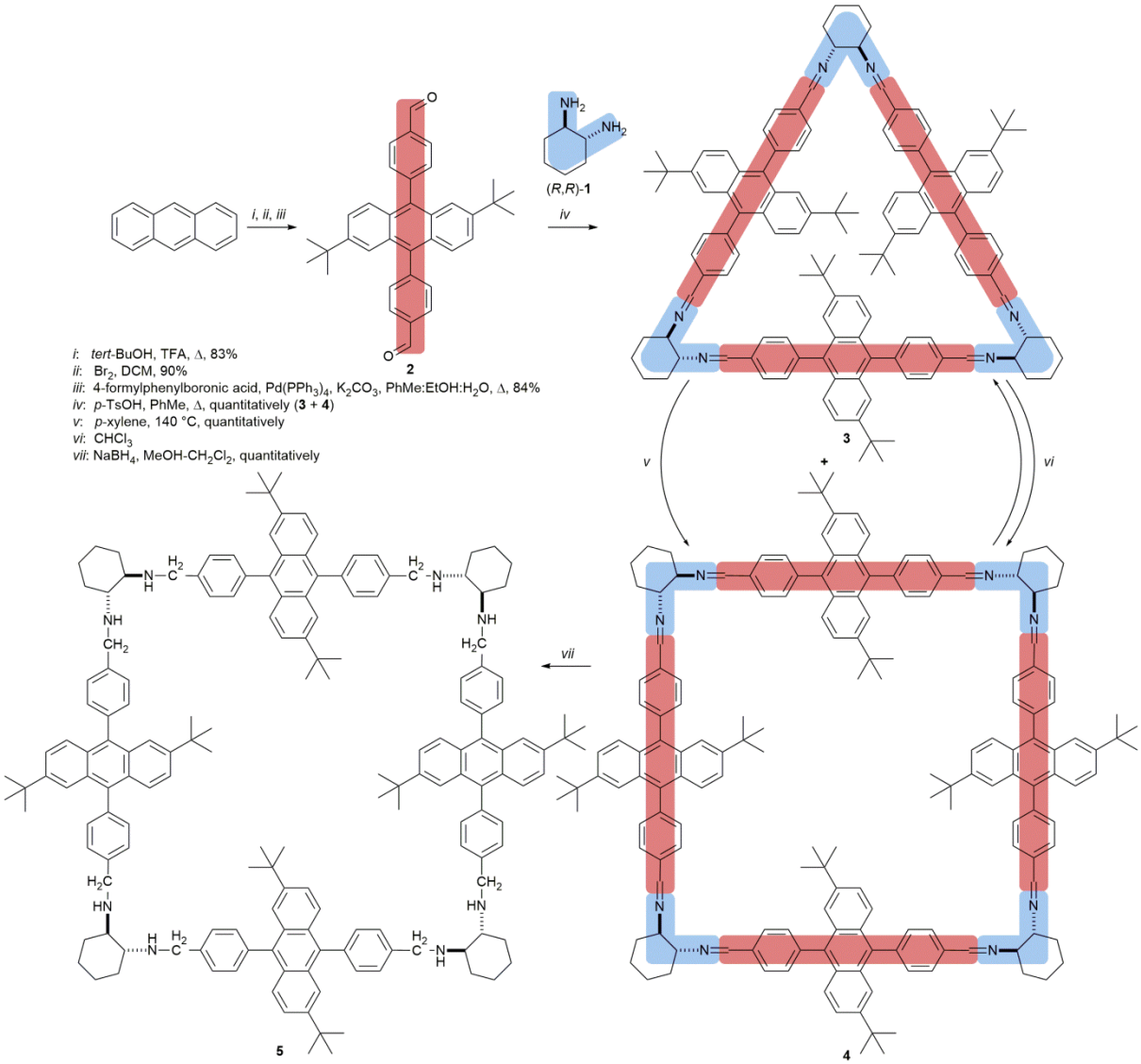


Scheme 1 (enlarged, alternate version).

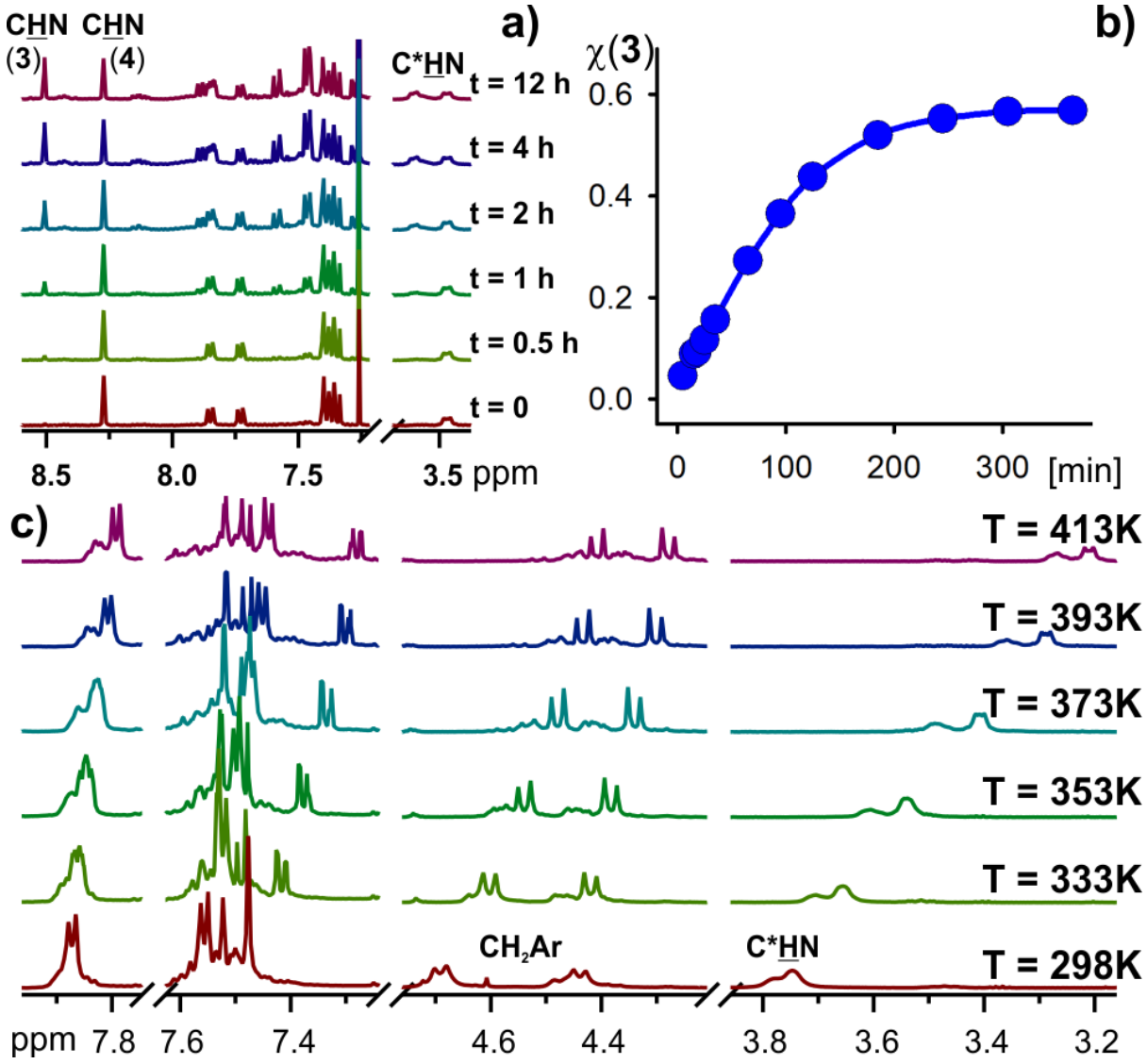


Figure 2 (enlarged version)

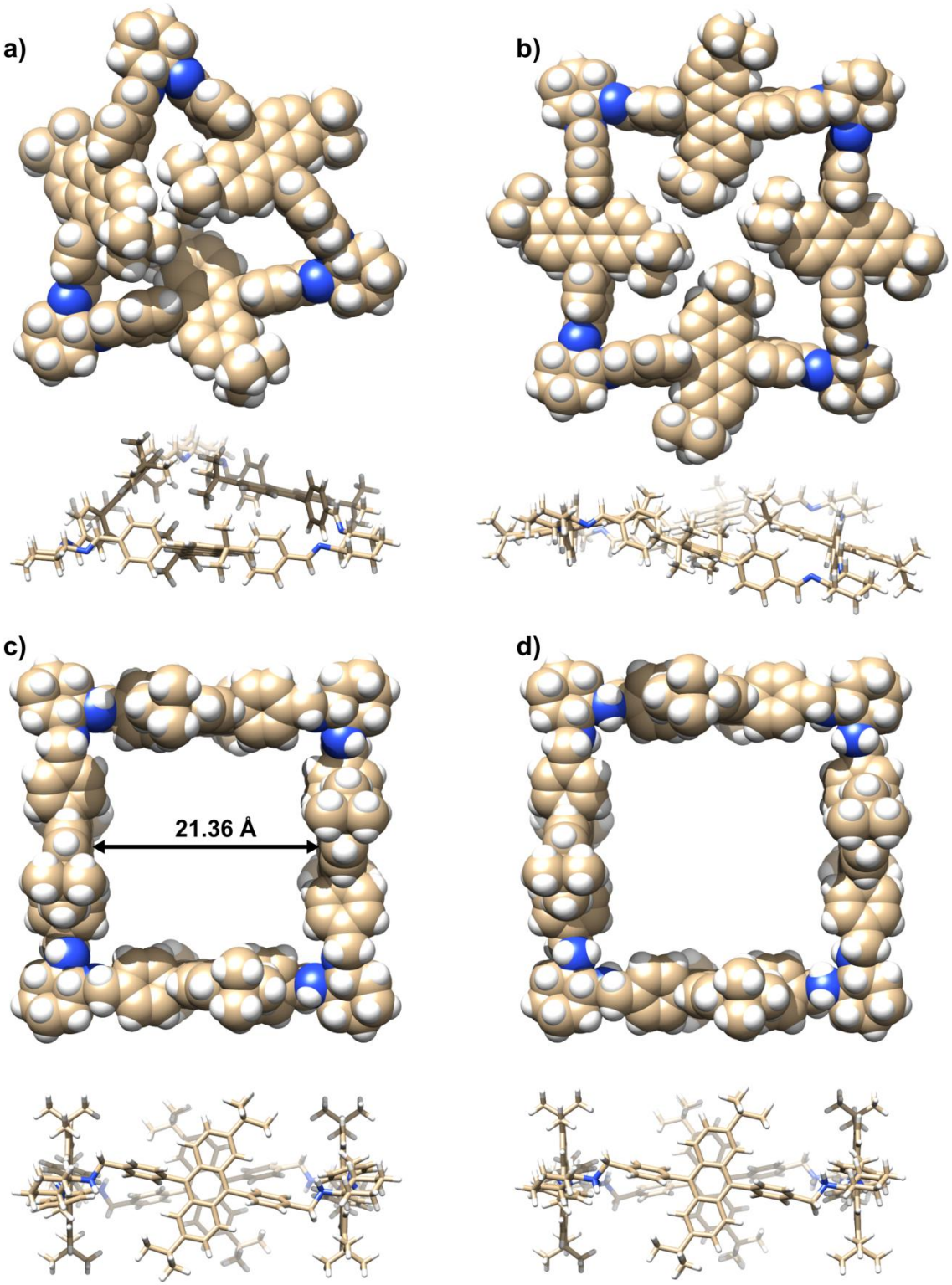


Figure 3 (alternate). Top and side views of low-energy structures of a) imine **3**; b) imine **4**; c) amine **5** and d) octaprotonated amine **5**×8H$^+$ calculated at the B3LYP/6-311G(d,p) level.

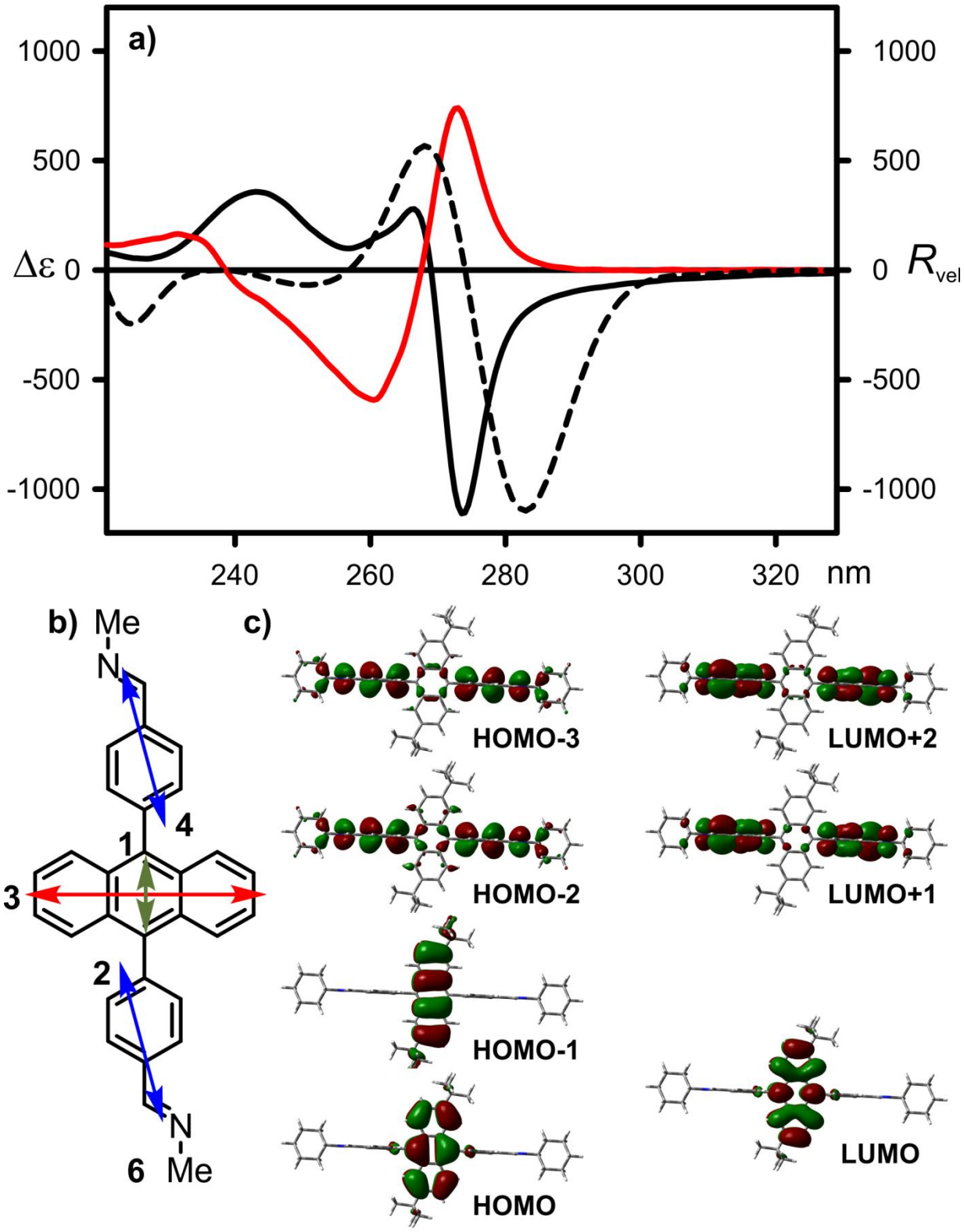


Figure 4 (enlarged version).

Experimental details

^{1}H and ^{13}C NMR spectra were recorded on Varian VNMR-S 400 MHz instrument. Chemical shifts (δ) are reported in ppm relative to $SiMe_4$ and coupling constants (*J*) are given in Hz. Mass spectra were run on AB Sciex Triple TOF 5600+ apparatus. UV and ECD spectra were recorded in spectroscopic grade chloroform using a JASCO J-810 instrument. Flash column chromatography was performed on Merck Kieselgel type 60 (250-400 mesh). Merck Kieselgel type $60F_{254}$ analytical plates were employed for TLC.

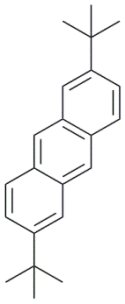
The time-dependent ^{1}H NMR spectra of imine **4** were recorded in $CDCl_3$, dried over calcium hydride. The pure imine **4** (10 mg) was dissolved in dry $CDCl_3$ (0.7 mL), quickly transferred to the test tube filled up with argon and the spectra were measured at certain time intervals (15 minutes).

The effect of the reaction conditions on the macrocyclization has been established by the comparison of the ^{1}H NMR spectra of the crude reaction mixtures. The equimolar amounts of both **1** and **2** were heated under reflux in appropriate solvent and with the use of Dean-Stark apparatus, for 12 hours. Then, all volatiles were evaporated to dryness. After having dissolved in dry $CDCl_3$, the crude product has been immediately analyzed by the ^{1}H NMR spectra measurements.

The surface areas and porosities of macrocyclic compounds were characterized by nitrogen adsorption and desorption analysis at 77.35 K with an autosorb computer controlled surface analyzer (ASAP 2420 Accelerated Surface Area and Porosimetry System, Micromeritics). Each sample was degassed at 70 °C for 72 h before analysis.

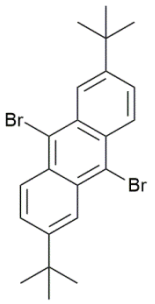
All known compounds were identified by spectroscopic comparison with authentic samples.

2,6-Di-*tert*-butylanthracene



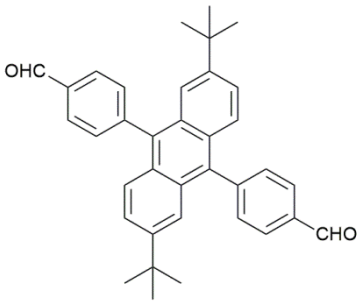
Obtained according to the previously described procedure.[S1]

9,10-Dibromo-2,6-di-*tert*-butylanthracene



Obtained according to the previously described procedure.[S2]

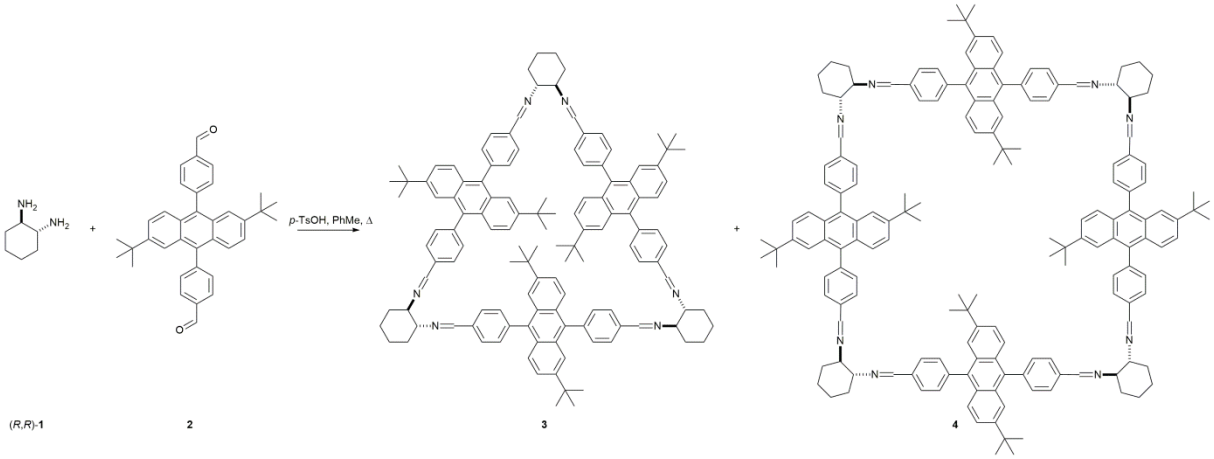
4,4'-(2,6-Di-tert-butylanthracene-9,10-diyl)dibenzaldehyde (**2**)



A mixture of 9,10-dibromo-2,6-di-*tert*-butylanthracene (4.109 g, 9.17mmol), 4-formylphenylboronic acid (4.440 g, 29.61 mmol), K_2CO_3 (14.665 g, 106.27 mmol) and $Pd(PPh_3)_4$ (0.610 g, 0.53 mmol) was added to degassed mixture of toluene/ethanol/water (55 mL/25 mL/20 mL) and the mixture was refluxed with stirring for 48 h under an argon atmosphere. After cooling, water (100 mL) was added and the mixture was extracted with dichloromethane. The collected organic extracts were dried over $MgSO_4$. After evaporation to dryness, the crude product was crystallized from mixture of hexane/ethanol. Yellow crystals of dialdehyde **2** were obtained with 84% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.23 (s, 2H), 8.15 (d, *J* = 8.2 Hz, 4H), 7.68 (d, *J* = 7.8 Hz, 4H), 7.56 (d, *J* = 9.1 Hz, 2H), 7.50 (d, *J* = 2.2 Hz, 2H), 7.46 (dd, *J* = 9.2, 1.9 Hz, 2H), 1.25 (s, 18H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 192.3, 147.8,

146.3, 135.7, 135.5, 132.3, 129.9, 129.2, 128.3, 126.2, 125.2, 120.8, 35.1, 30.9. HRMS (m/z) calculated for $C_{36}H_{34}O_2$ 498.2559, found [M+H+] 499.2645.

Cyclocondensation reaction between (*R*,*R*)-**1** and **2**



A mixture of dialdehyde **2** (0.993 g, 2.00 mmol), (*R*,*R*)-1,2-diaminocyclohexane (0.229 g, 2.00 mmol), catalytic amounts of *p*-toluenesulfonic acid (0.011 g, 0.06 mmol) and toluene (100 mL) were placed in a round-bottom flask (under argon). The mixture was heated with stirring using Dean–Stark apparatus for one day. The solution was cooled to ambient temperature and the solvent was removed under reduced pressure to give mixture of macrocycles **3** and **4** in almost quantitative yield.

Macrocycle **4**

The crude mixture of macrocycles **3** and **4** was heated in *p*-xylene for 1h and then solvent was evaporated yielding pure [4+4] macrocycle as only product. ^{1}H NMR (600 MHz, $CDCl_3$ + Et_3N) δ 8.27 (s, 8H), 7.85 (dd, *J* = 7.9, 1.7 Hz, 8H), 7.73 (dd, *J* = 7.8, 1.7 Hz, 8H),7.40-7.35 (m, 32H), 6.92 (dd, *J* = 9.2, 2.0 Hz, 8H), 3.46 (m, 8H), 2.14 (m, 8H), 1.97 (m, 16H), 1.60 (m, 8H), 0.82 (s, 72H). ^{13}C NMR (75 MHz, $CDCl_3$ + Et_3N) δ 162.7, 146.9, 141.8, 135.8, 135.3, 131.5, 129.2, 128.4, 128.2, 127.7, 126.2, 124.6, 73.7, 34.6, 30.8, 30.8, 30.6, 11.7. HRMS (m/z) calculated for $C_{168}H_{176}N_8$ 2306.4052, found [$M+H^+$] 2307.4105.

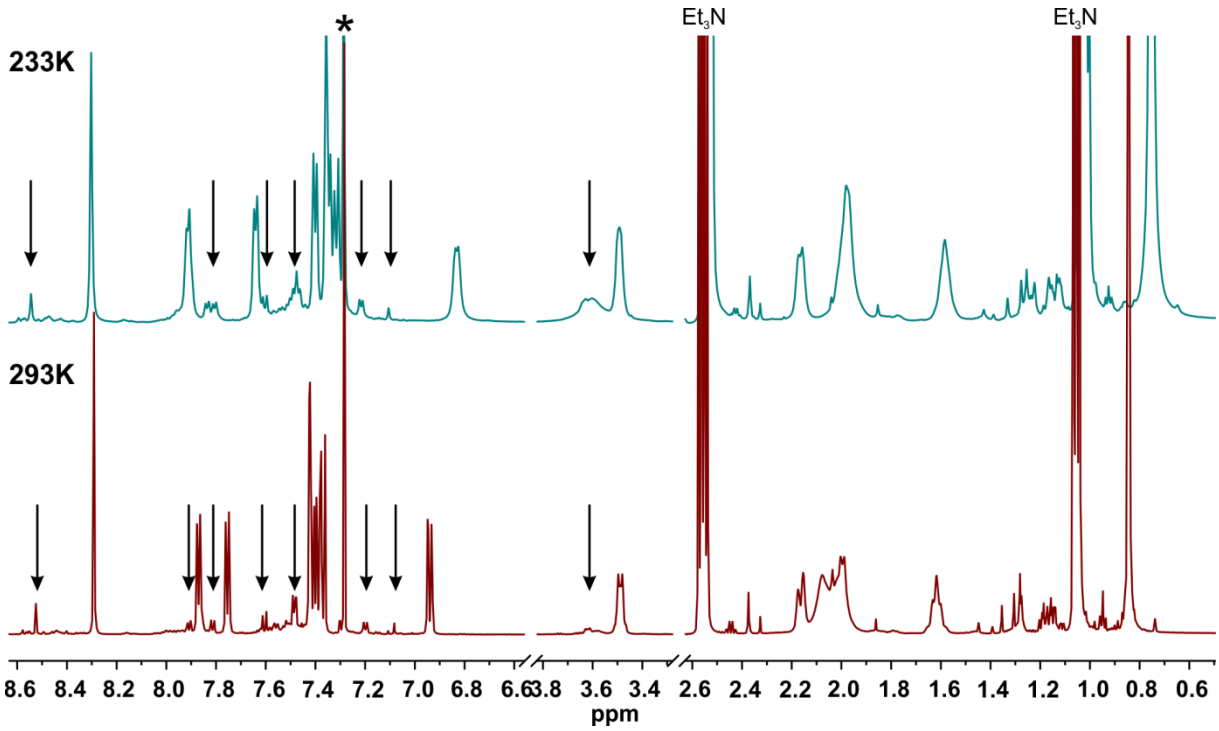
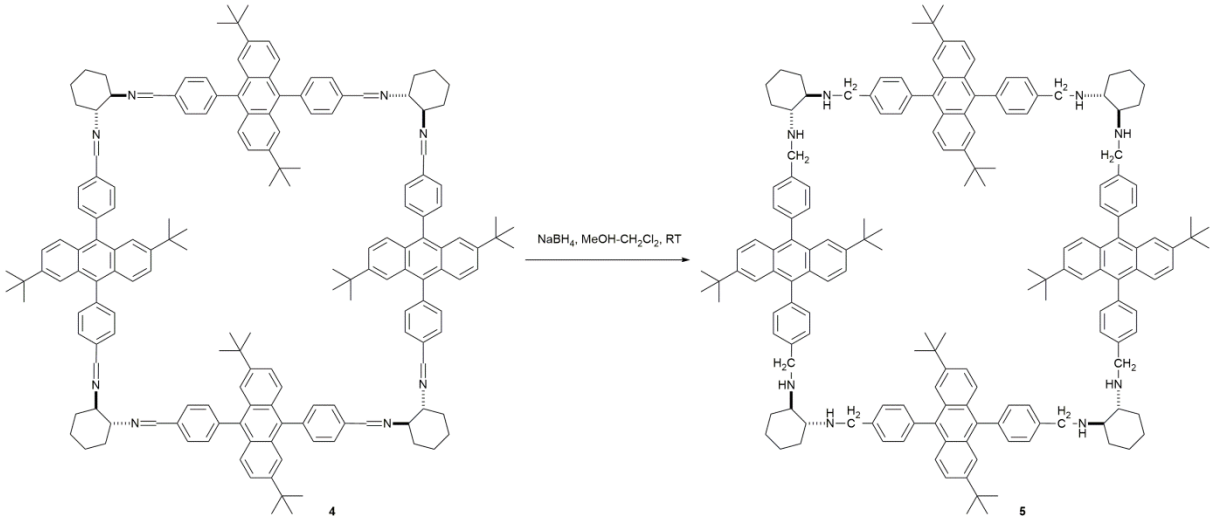


Figure S1. Traces of ^{1}H NMR spectra of **4** measured in $CDCl_3$ containing drop of triethylamine at room temperature (lower panel) and at -40 °C (upper panel). Arrows, seen in the diagnostic region of spectrum, indicate signals originated from [3+3] macrocycle **3**. Although the spectra were measured as soon as the sample was dissolved, the formation of macrocycle **3** is visible. Below temperature -40 °C the macrocycle precipitated, which prevented further measurements.

Macrocycle **5**



Mixture of macrocycle **4** (1.120 g, 0.48 mmol) and K_2CO_3 (0.104 g, 106.27mmol) was dissolved in $CHCl_3$/MeOH (50 mL/50 mL) and cooled in ice bath to 0 °C, then $NaBH_4$ (1.520 g, 40.00 mmol) was added in small portions. After stirring for one day at RT, water (50 mL) was added and mixture was extracted with 10% K_2CO_3 water solution. The organic layer was dried over Na_2SO_4, filtered through pad of celite and evaporated to dryness to give pure macrocycle **5** with 87% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, *J* = 9.3 Hz, 8H), 7.57 (m, 16H), 7.52 (d, *J* = 2.0 Hz, 8H), 7.39 (m, 16H), 7.26 (dd, *J* = 9.2, 2.0 Hz, 8H), 4.02 (dd, *J* = 142.4, 13.2 Hz, 16H), 2.50 (m, 8H), 2.37 – 2.27 (m, 8H), 2.11 (m, 8H), 1.84 (m, 8H), 1.39 – 1.31 (m, 8H), 1.09 (s, 72H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.6, 140.0, 138.0, 136.2, 131.5, 129.7, 128.4, 128.0, 126.6, 124.3, 121.2, 61.1, 50.9, 34.9, 31.8, 30.9, 30.8, 25.3. HRMS (m/z) calculated for $C_{168}H_{192}N_8$ 2322.5304, found [M+H$^+$] 2323.5361.

Calculation details

The initial molecular geometries of possible isomers of **3**-**5** were generated with the use of SCIGRESS software (MM3 force field), by rotation around all rotatable single bonds.[S2] Then, the obtained initial structures were pre-optimized at the semiempirical PM6 level.

The structure of individual isomers of **3**-**5** were fully optimized at the B3LYP/6-311G(d,p) level. For each calculated low-energy structure the single-point energy at the B3LYP-GD3BJ/6-311G(d,p) level was calculated.[S3,S4]

The model compound **6**, being the fourths of the macrocycle **4**, was extracted from mother molecule and then optimized at the B3LYP/6-311G(d,p) level. For optimized structure of **6**, characterized by C_i symmetry, the UV spectrum was calculated at the CAM-B3LYP/6-311G(d,p) level.

Since the size of the systems did not allow for reliable TD-DFT calculations, the ECD spectra for **4** and **5** were calculated at the semi-empirical ZINDO level.

All UV and ECD spectra were simulated by overlapping Gaussian functions for each transition, according to the procedure previously described by Harada and Stephens.[S5]

All calculations were performed for molecules in the gas phase.

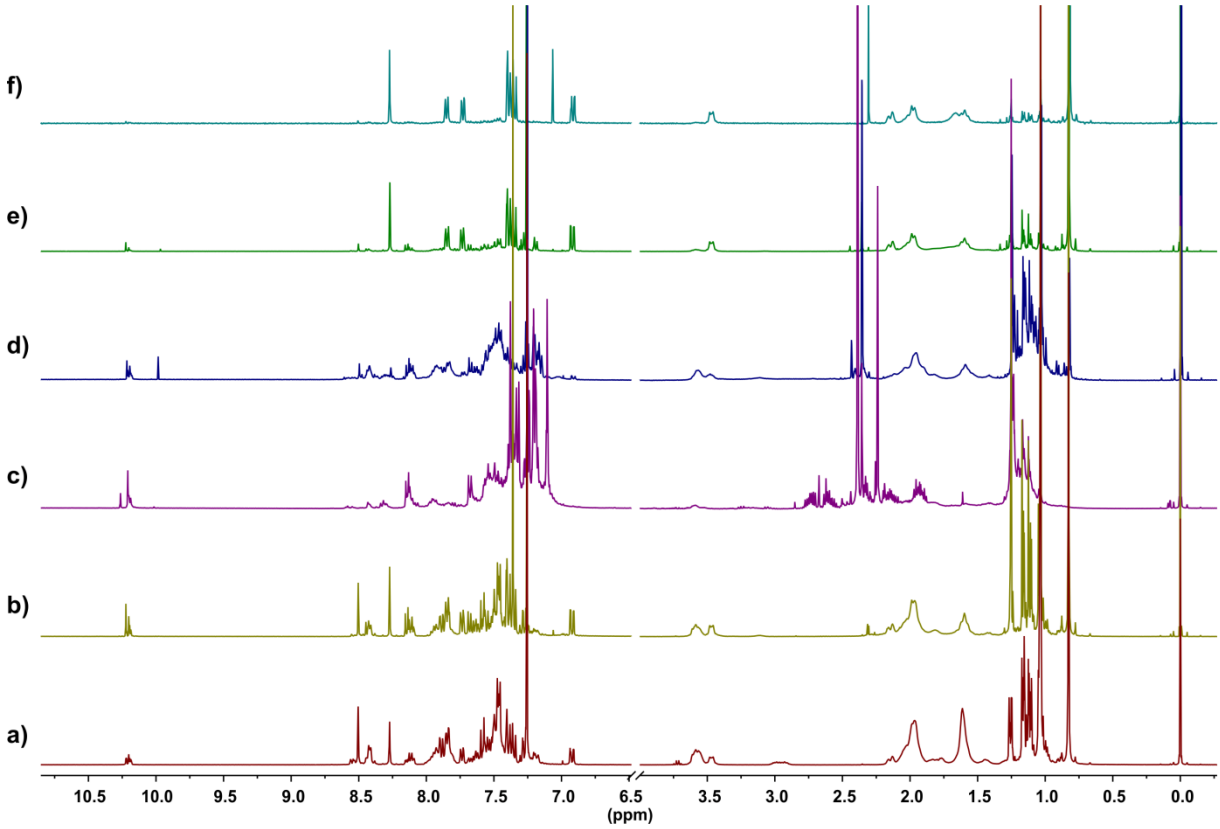


Figure S2. a) Traces of ^{1}H NMR spectra [$CDCl_3$] measured for crude products of reactions between equimolar amounts of **1** and **2** and carried out in different solvents: a) chloroform (RT); b) benzene (reflux); c) *o*-xylene (110 °C); d) *m*-xylene (110 °C); e) *p*-xylene (110 °C); f) toluene, then *p*-xylene (reflux).

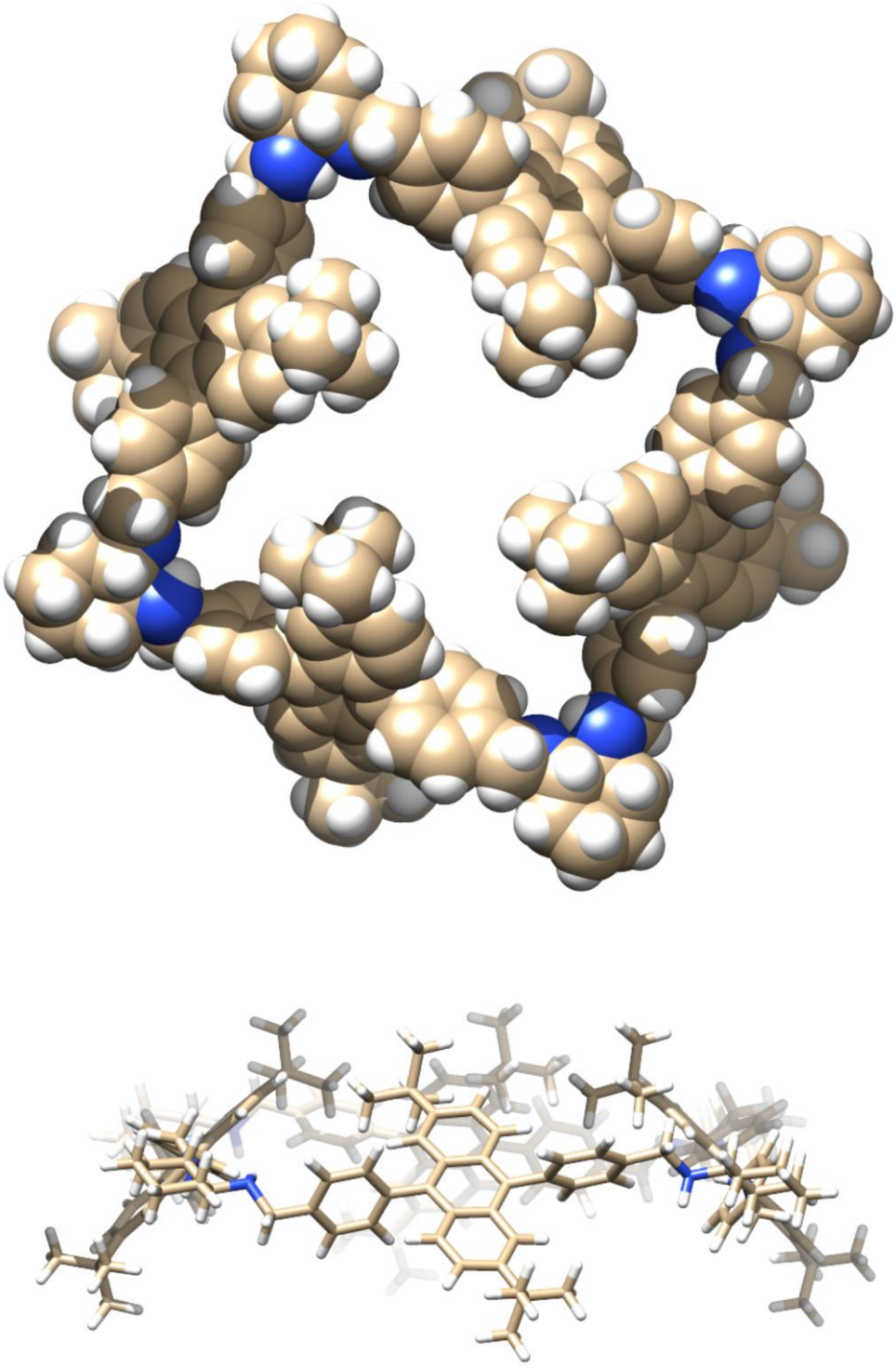


Figure S3. Top and side view of the bowl-shaped conformer of **5** optimized at the B3LYP/6-311G(d,p) level.

Interpretation of ECD spectra of 4 and 5 in terms of exciton chirality rule

The exciton chirality method (ECM) requires at least two chromophores characterized by strong UV absorption in a given spectral region and well-defined orientation of electronic transition dipole moment(s) (ETDM(s)). Thus, the geometrical relationship between interacting ETDMs μ_i and μ_j (so called – coupled oscillators) can be easily related to the absolute configuration and/or conformation of a given molecular system. The sign of exciton couplet is the function of dihedral angle ω between interacting EDTMs (strictly speaking is the function of the sine of the angle ω). In general, if the two interacting chromophores constitute a clockwise screw sense, the ECD shows a positive first CE at longer wavelength and a negative second CE at shorter wavelength and *vice versa*. The intensity of the exciton CD (A value) is inversely proportional to the square of the interchromophoric distance R_{ij}.[S6]

For molecular systems containing more than two chromophores the observed exciton couplet in a given spectral region is a sum of contributions from interacting pairs of chromophores (A/B, B/C, C/A, etc.).[S6]

To start the study, we determined polarization of the main electronic transitions within chromophores. In Figure S3 we showed UV spectra, polarizations of electronic transitions of the highest oscillator strengths and orbitals mainly involved in electronic transitions, calculated for model chromophoric system **6**.

The results obtained for model compounds were further used for the interpretation of CD spectrum of **4** in terms of excitons. The macrocycles were divided into individual, namely imine ($C_6H_4CH=N$) and anthracene chromophores (see Figure S4). In the case of **4**, there are 12 sub-units (A-L), 8 imine and 4 anthracene. The midpoints (M_{Ar}) of the aromatic rings were taken as origins of respective electric dipoles, whereas the midpoints of C=N ($M_{C=N}$) and C2=C3 ($M_{C=C}$ in anthracene) bonds were taken as the end points of respective dipoles. The angle ω_1 is defined here as M_{Ar}-$M_{C=N}$-$M_{C=N}$-M_{Ar}, the angle ω_2 is defined as $M_{C=C}$-M_{Ar}-M_{Ar}-$M_{C=C}$ and the angle ω_3 is defined as M_{Ar}-$M_{C=N}$-M_{Ar}-$M_{C=C}$. The intrachromophoric interactions (namely, imine-anthracene) were not taken into considerations. The structural parameters important for the interpretation of CD spectra in terms of excitons were collected in Table S_1.

To estimate more quantitatively the contribution of the particular molecular fragment to the overall rotatory strength and therefore to the CE we divided macrocycle **4** into two fragments: imine and anthracene. For each fragment the UV and ECD spectra were calculated at the TD-CAM-B3LYP/6-311G(d,p) level. The results were shown in Figure S5.

Since we were not able to calculate ECD spectrum of **4** at sufficiently high level of DFT theory, the absorption and CD spectra of this particular macrocycle and of the macrocycle **5** were calculated at ZINDO level (Figures S6 and S7).

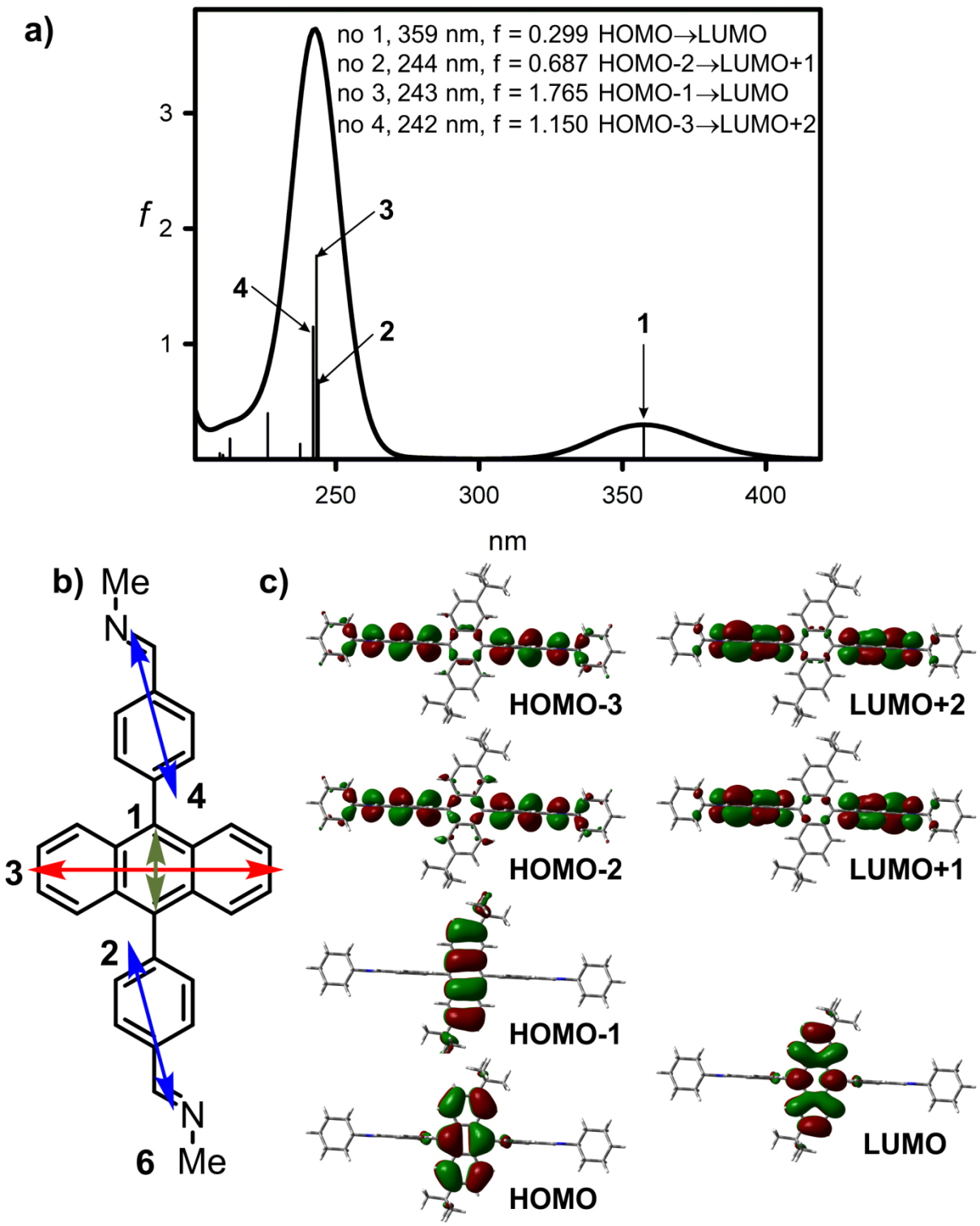


Figure S4. a) UV spectra, b) directions of polarization of main electronic transitions calculated at the TD-CAM-B3LYP/6-311G(d,p) level for model chromophoric system **6**. Vertical bars represent calculated oscillator strengths. The calculated spectrum was not wavelength corrected. Insert shows energies, oscillators strengths and orbitals mainly contributed to a given electronic transition. c) Visualization of orbitals involved in the main electronic transition within chromophore **6**.

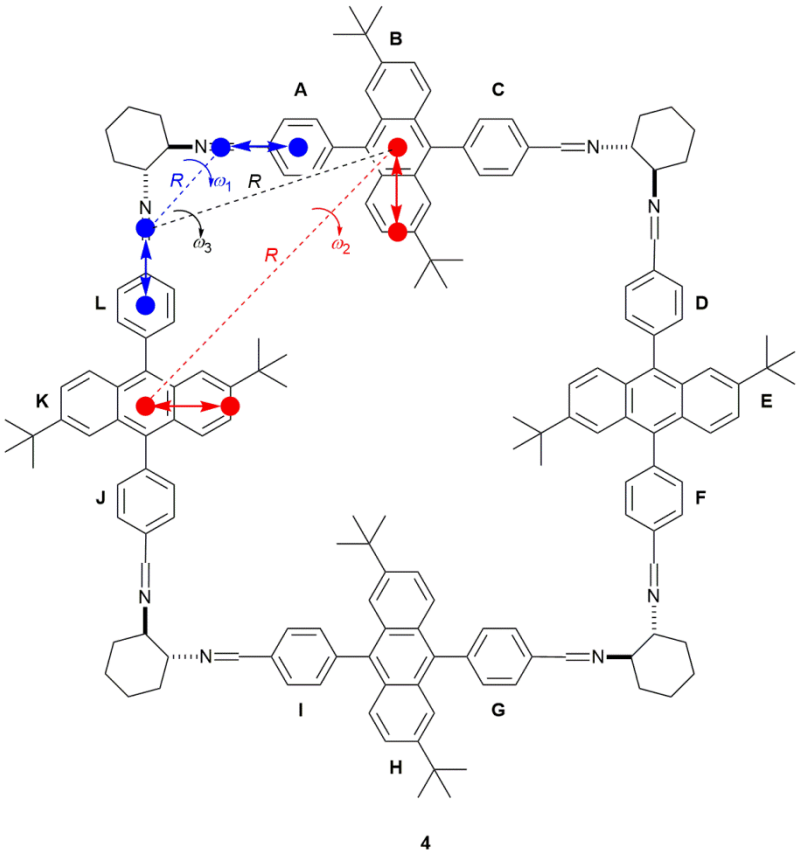


Figure S5. Way of dividing the molecule **4** into chromophoric fragments, schematic representation of EDTMs important for analysis of ECD spectrum and definitions of angles ω_1-ω_3 and interchromophoric distances R_{ij}.

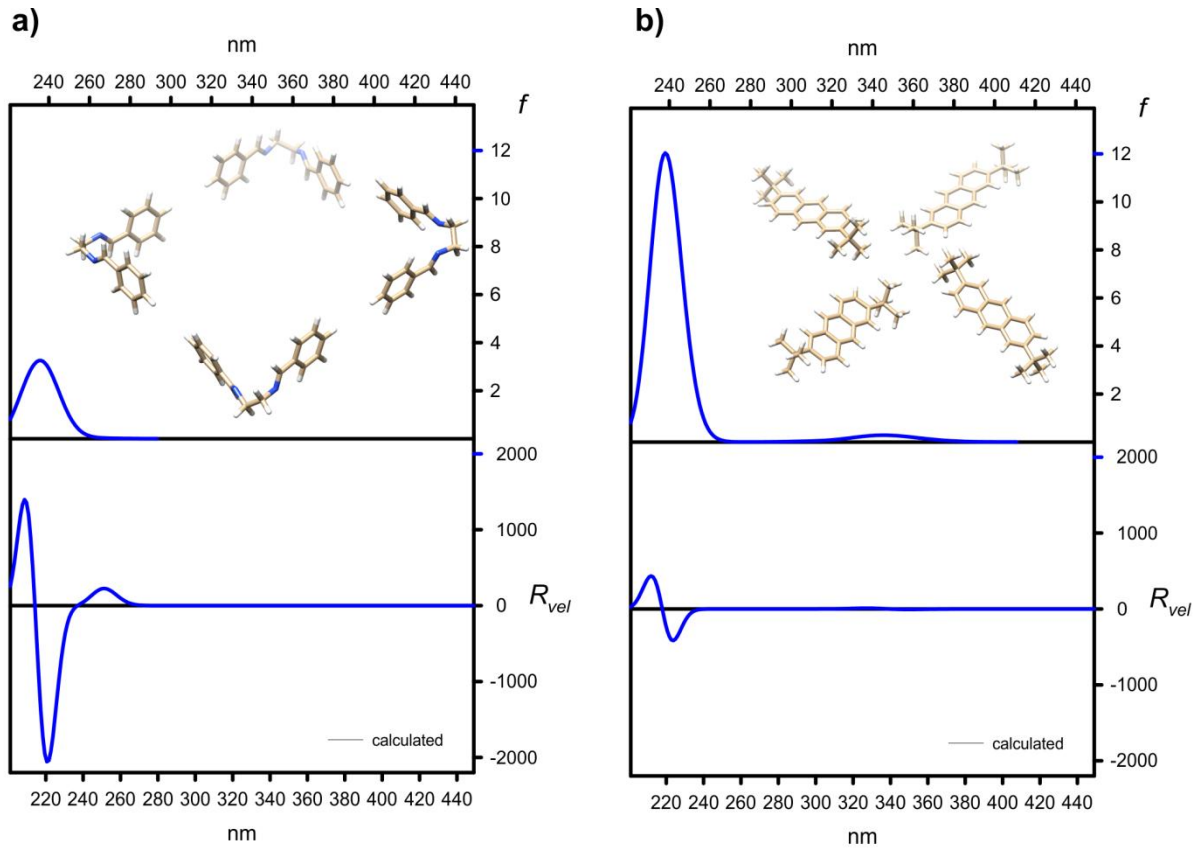


Figure S6. UV (upper panels) and ECD (lower panels) spectra of a) "imine" and b) "anthracene" fragments of the molecule **4**, calculated at the TD-CAM-B3LYP/6-311G(d,p) level. Wavelengths were not corrected. Inserts show particular molecular fragment for which calculations were carried out.

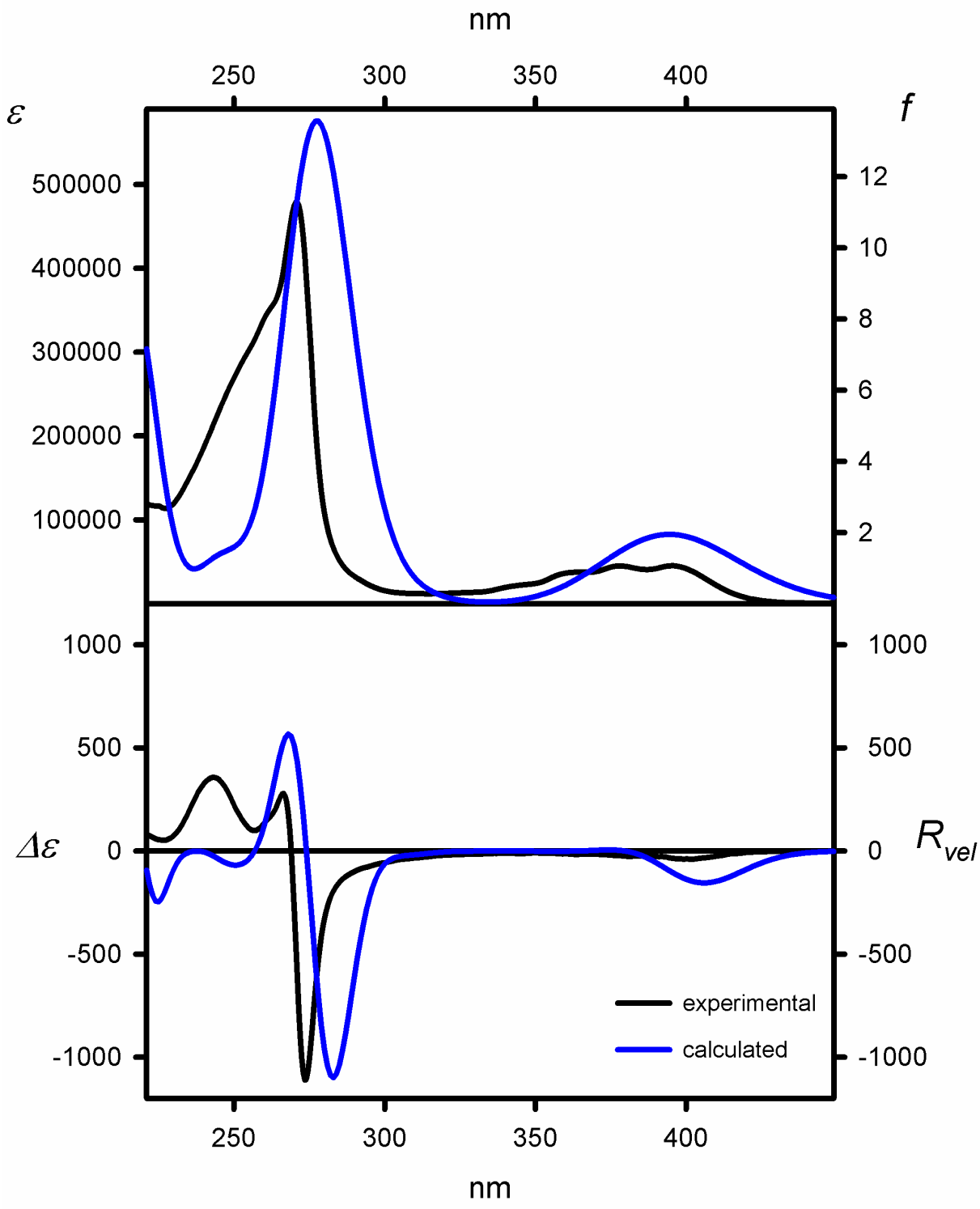


Figure S7. UV (upper panels) and ECD (lower panels) spectra of **4**, experimental, measured in dichloromethane (black lines) and calculated at the ZINDO level (blue lines). Wavelengths were not corrected.

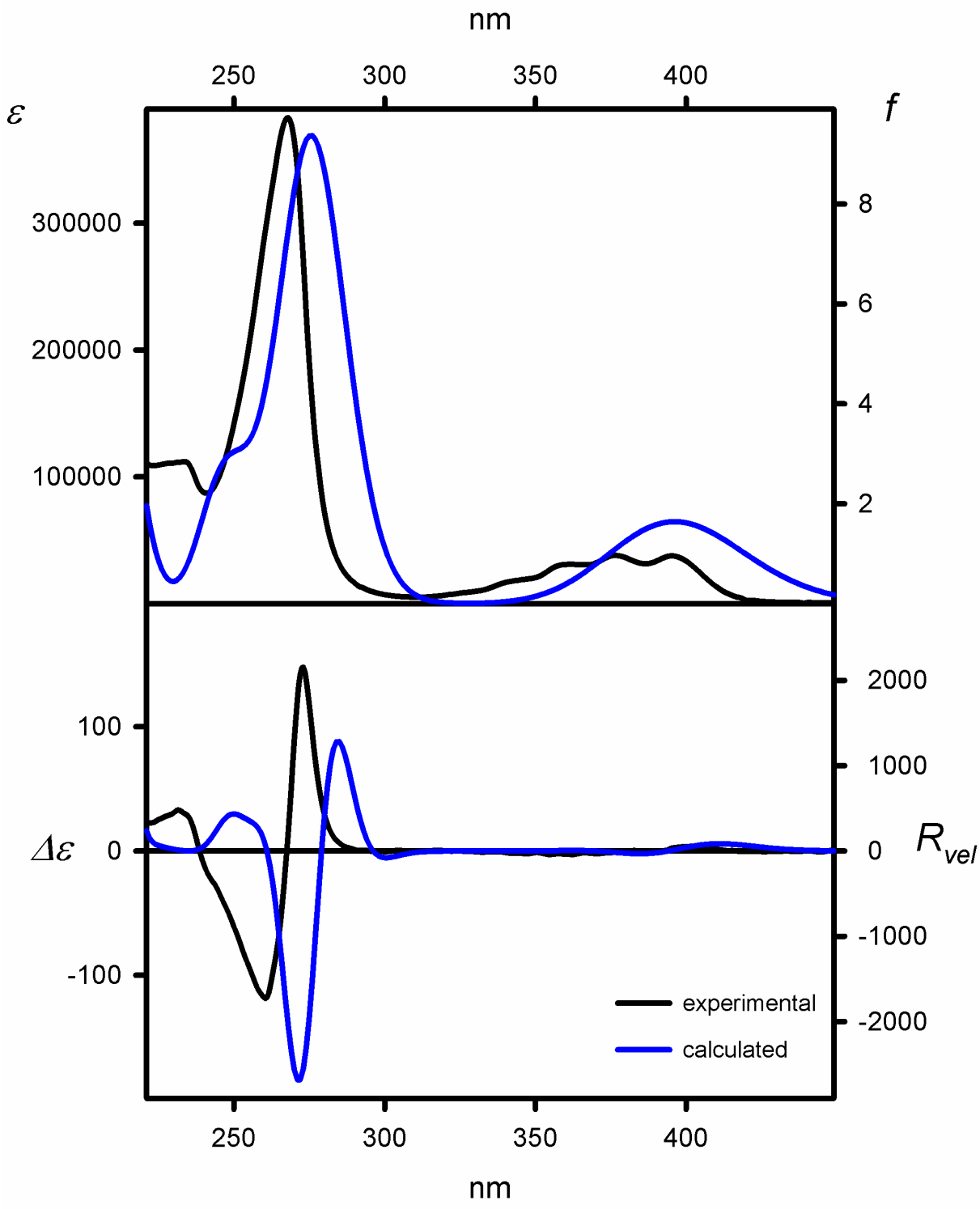
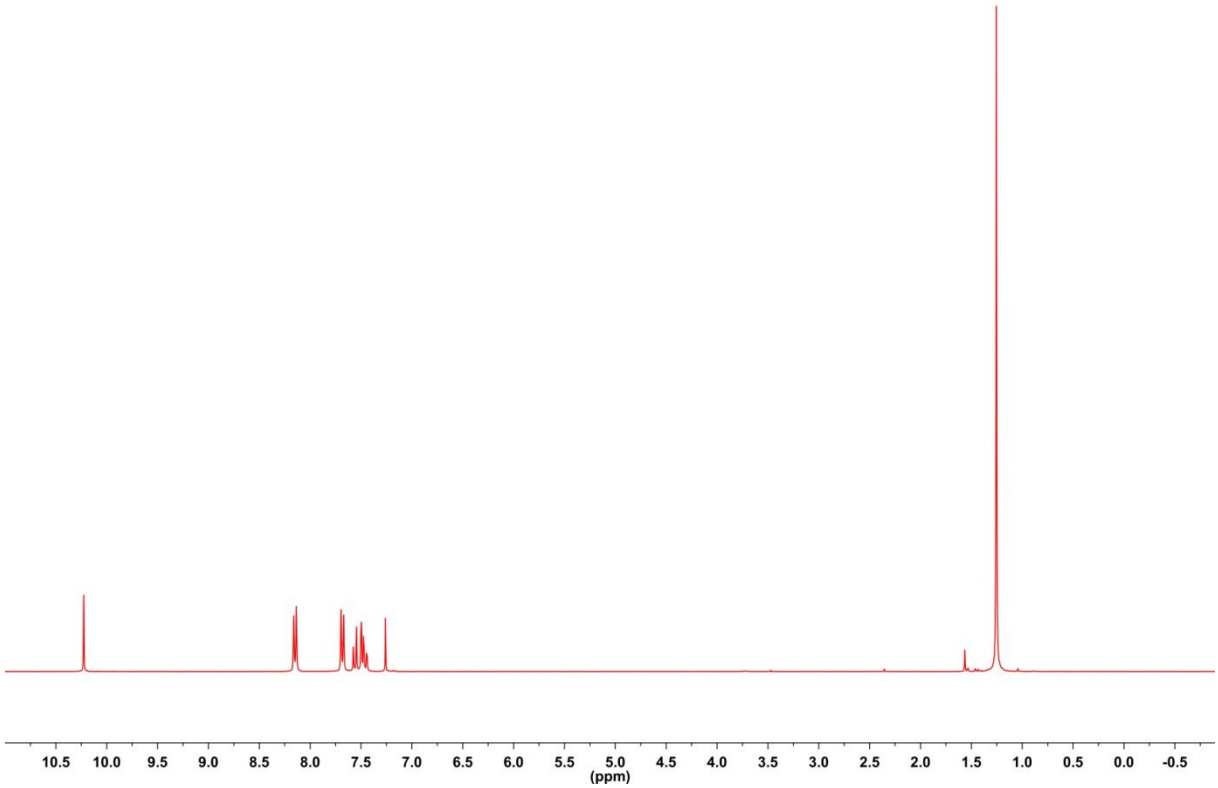


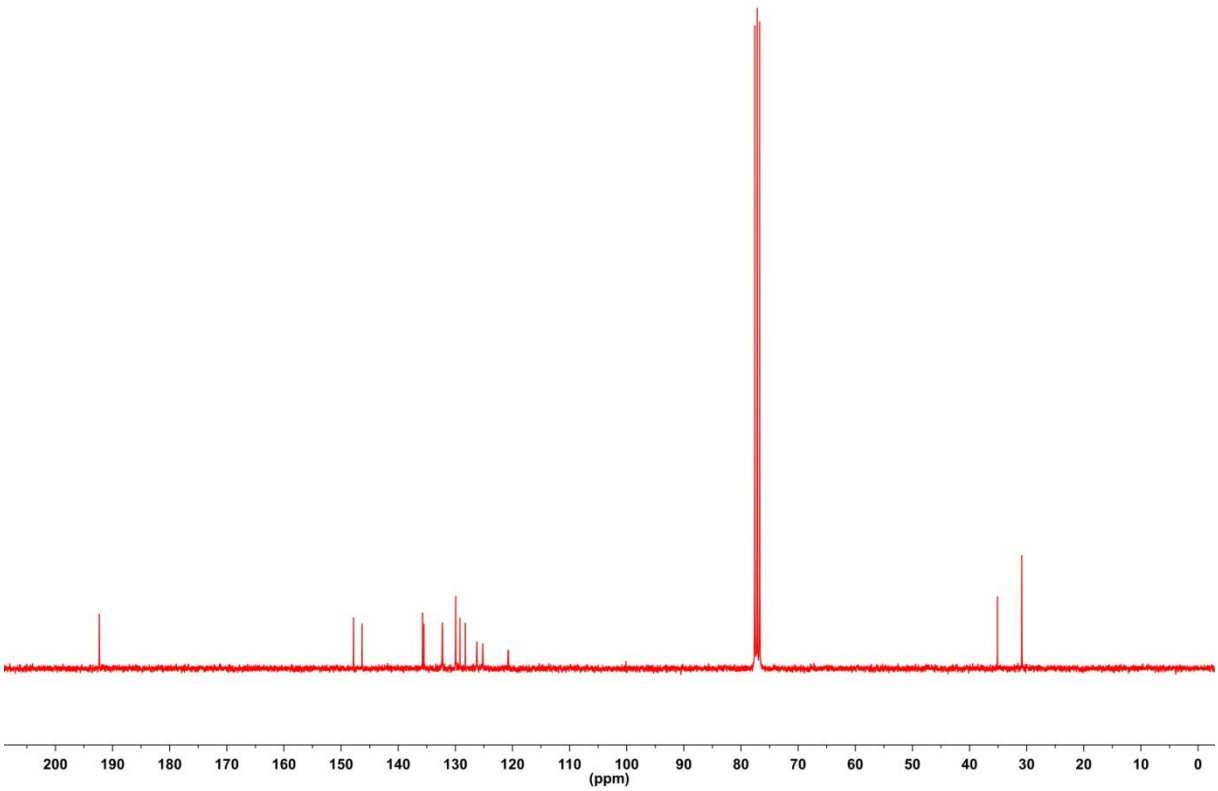
Figure S8. UV (upper panels) and ECD (lower panels) spectra of **5**, experimental, measured in dichloromethane (black lines) and calculated at the ZINDO level (blue lines). Wavelengths were not corrected.

Table S_1. Torsion angles ω_1-ω_3, interchromophoric distances R_{ij} between each pair of interacting chromophores A-L and estimated amplitudes of exciton Cotton effects for particular interaction.

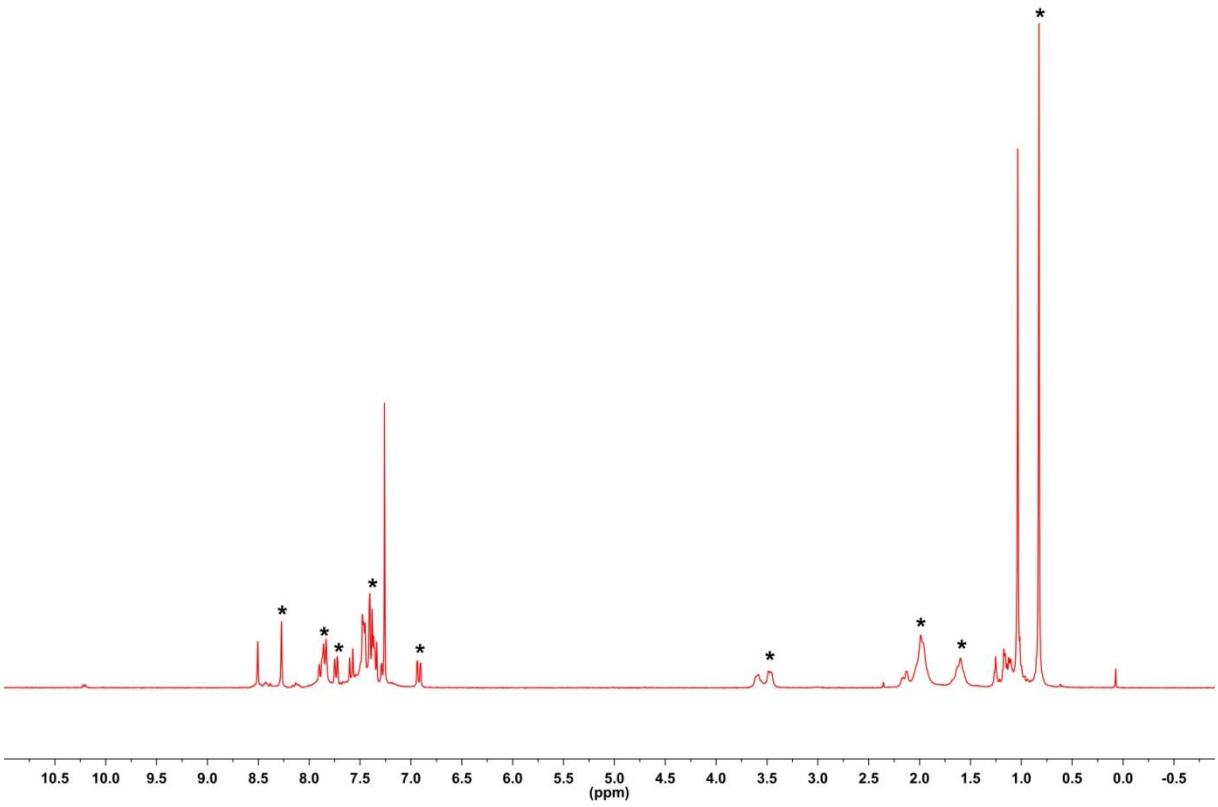
Interchromophoric interaction	Angle ω_1 [°]	Angle ω_2 [°]	Angle ω_3 [°]	Iterchromophoric distance R_{ij} [Å]	Sign of exciton CE
A-L	-24.7			3.48	-
C-D	-25.1			3.51	-
F-G	-25.7			3.50	-
I-J	-26.1			3.50	-
B-E		-22.0		13.46	-
E-H		22.5		13.30	+
H-J		-24.1		13.43	-
J-B		23.3		13.20	+
B-H		-65.8		18.99	-
E-J		-0.7		18.76	~0
A-K			6.05	10.68	+
B-L			12.8	10.84	+
B-D			3.9	10.94	+
C-E			-17.9	10.94	-
E-G			6.03	10.76	+
F-H			12.5	10.90	+
H-J			5.2	10.87	+
I-K			-21.2	10.94	-

Copies of ^{1}H and ^{13}C NMR spectra.

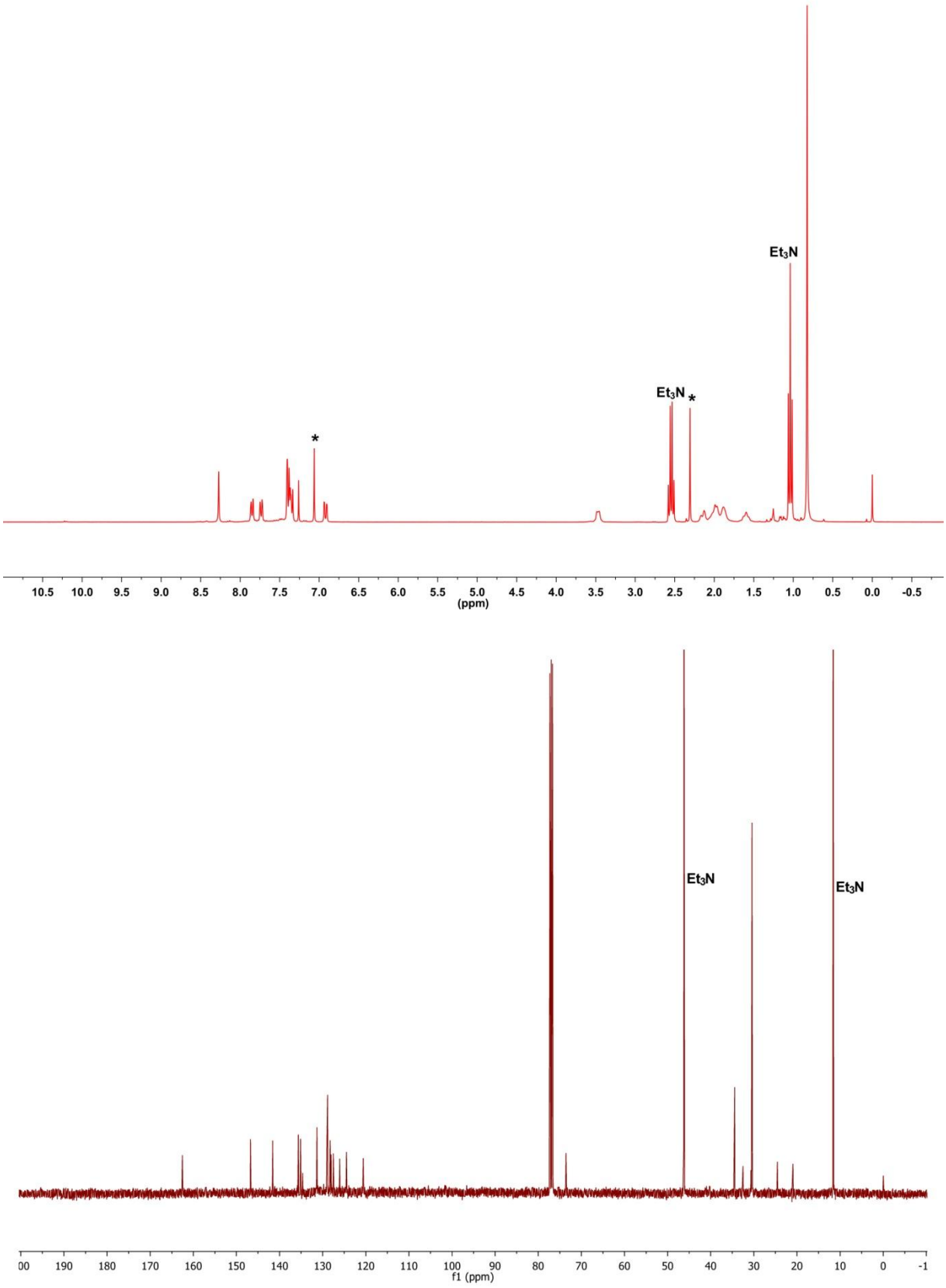




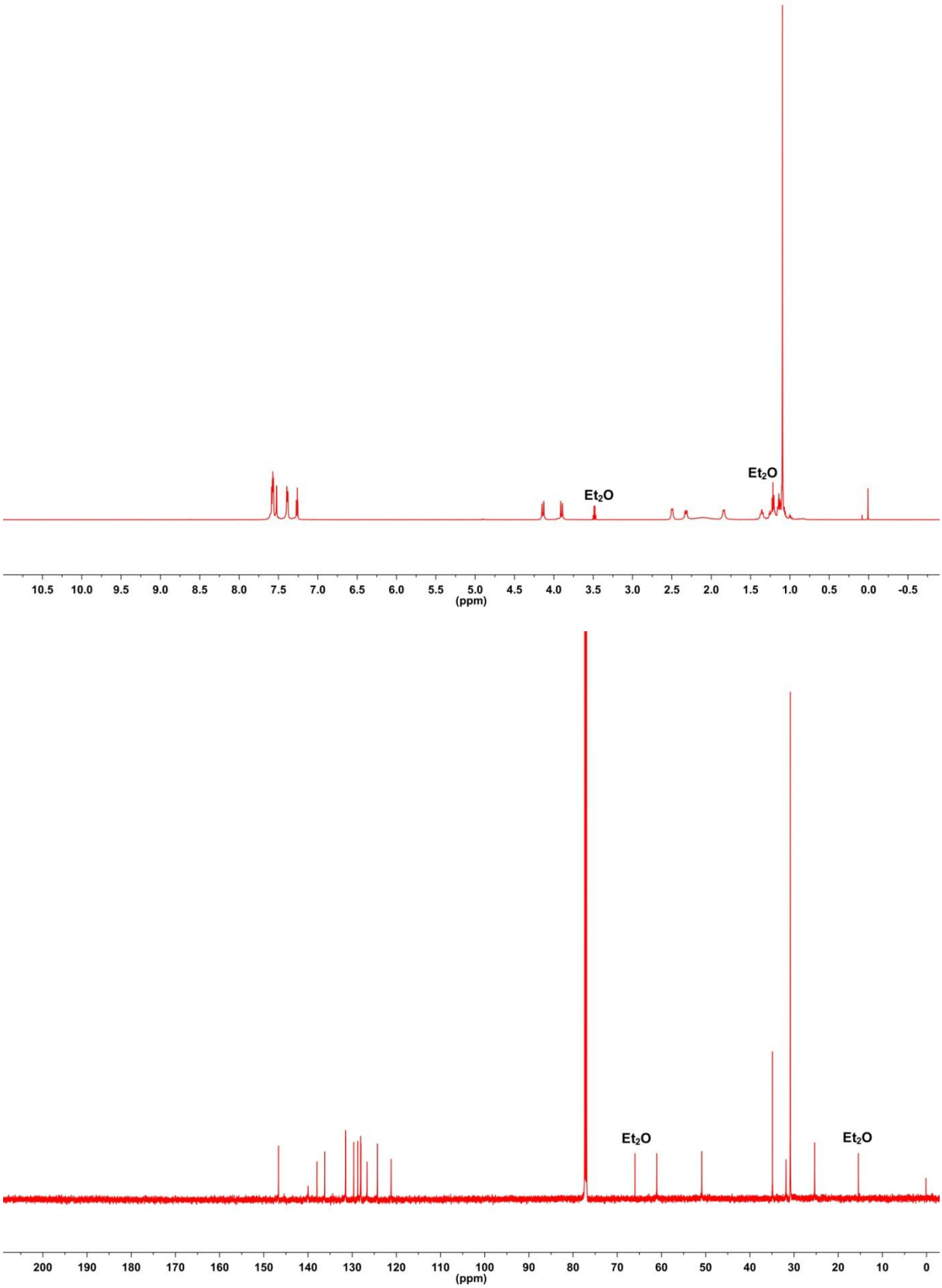
^{1}H (upper panel) and ^{13}C NMR (lower panel) spectra of aldehyde **2**.



^{1}H NMR spectrum measured for crude mixture of **3** and **4**. Asterisks indicate peaks originated from [4+4]-**4**.



^{1}H NMR (upper panel) and ^{13}C NMR (lower panel) spectra of **4**. Asterisks indicate *p*-xylene.



^{1}H NMR (upper panel) and ^{13}C NMR (lower panel) spectra of **5**.

Cartesian coordinates

3	1	6	0	-2.934591	10.587629	0.974717
	2	6	0	-1.700121	10.967368	0.127581
	3	6	0	-4.080643	11.589116	0.724596
	4	6	0	-1.271344	12.418641	0.409221
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	12	6	0	3.098269	6.565164	-0.112233
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	17	6	0	4.136319	5.497140	0.035255
	18	6	0	3.750209	4.224284	0.503288
	19	6	0	5.478498	5.741437	-0.310564
	20	6	0	4.727646	3.171376	0.601561
	21	6	0	6.462265	4.693731	-0.196007
	22	6	0	6.072527	3.414633	0.251995
	23	6	0	2.396453	3.943742	0.877026
	24	6	0	1.986917	2.715041	1.323632
	25	6	0	4.268533	1.889460	1.041579
	26	6	0	2.966921	1.674484	1.388283
	27	6	0	5.924843	7.019244	-0.771506
	28	6	0	7.231977	7.248789	-1.086055
	29	6	0	7.823224	4.992836	-0.529201
	30	6	0	8.228194	6.227309	-0.967643
	31	6	0	7.066088	2.302532	0.361402
	32	6	0	7.520047	1.873702	1.613458
	33	6	0	7.523833	1.626284	-0.781034
	34	6	0	8.377594	0.783938	1.722443
	35	6	0	8.385361	0.543652	-0.674679
	36	6	0	8.813799	0.098417	0.583571
	37	6	0	9.674723	-1.085414	0.738352
	38	6	0	0.542811	2.417526	1.748871
	39	6	0	9.684970	6.557335	-1.326700
	40	6	0	2.677730	-5.835891	-0.598011
	41	6	0	1.706122	-4.902646	-1.023888
	42	6	0	2.271876	-7.056883	-0.021632
	43	6	0	0.301770	-5.193867	-0.873195
	44	6	0	0.866993	-7.333988	0.154057
	45	6	0	-0.100794	-6.404422	-0.267670
	46	6	0	2.053863	-3.642367	-1.596750
	47	6	0	1.104108	-2.760640	-2.034423
	48	6	0	-0.648319	-4.236360	-1.342302
	49	6	0	-0.289215	-3.047281	-1.931212
	50	6	0	3.220259	-8.056021	0.376250

	51	6	0	2.853128	-9.251496	0.936772
	52	6	0	0.510024	-8.586625	0.747458
	53	6	0	1.454078	-9.495406	1.122869
	54	6	0	-1.556379	-6.691949	-0.068481
	55	6	0	-2.176874	-6.403686	1.151541
	56	6	0	-2.334004	-7.245857	-1.097606
	57	6	0	-3.532715	-6.659099	1.337587
	58	6	0	-3.687029	-7.496168	-0.915883
	59	6	0	-4.306815	-7.203462	0.307306
	60	6	0	-5.742388	-7.455871	0.526831
	61	6	0	-1.369572	-2.078939	-2.451604
	62	6	0	3.862864	-10.330016	1.357558
	63	6	0	10.993306	-2.890068	0.063485
	64	6	0	10.494641	-4.099484	-0.758174
	65	6	0	12.467233	-2.591163	-0.267000
	66	6	0	11.389050	-5.326461	-0.500547
	67	6	0	13.364525	-3.812046	-0.029075
	68	6	0	12.862947	-5.034389	-0.808124
	69	7	0	10.177768	-1.723944	-0.237067
	70	7	0	9.121701	-4.415092	-0.392792
	71	6	0	8.279981	-4.566144	-1.331492
	72	6	0	6.862640	-4.901498	-1.114767
	73	6	0	4.130005	-5.527039	-0.773819
	74	6	0	4.708228	-5.515130	-2.048321
	75	6	0	4.946598	-5.226568	0.328967
	76	6	0	6.052645	-5.199889	-2.215756
	77	6	0	6.290999	-4.923520	0.164912
	78	6	0	-7.917067	-8.112775	-0.067727
	79	6	0	-8.805469	-7.167599	-0.918510
	80	6	0	-8.242981	-9.588157	-0.365690
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	86	6	0	-8.024149	-4.983580	-1.276809
	87	6	0	-7.757939	-3.577568	-0.925601
	88	6	0	-7.145444	-0.903493	-0.255926
	89	6	0	-6.656932	-1.477562	-1.435440
	90	6	0	-7.968180	-1.684750	0.571322
	91	6	0	-6.964206	-2.792979	-1.768413
	92	6	0	-8.265316	-3.001145	0.247486
	93	6	0	-6.766757	0.496814	0.107638
	94	6	0	-5.838979	0.732853	1.145437
	95	6	0	-7.311164	1.584042	-0.605513
	96	6	0	-5.402453	2.078938	1.423013
	97	6	0	-6.890551	2.931467	-0.315713
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	151	1	0	8.705355	0.453689	2.703385
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165	1	0	13.381598	-4.048098	1.042403
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187	1	0	-6.568818	-3.222124	-2.683751
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194	1	0	-8.807440	6.535838	-1.263277
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79	1	0	4.730857	-11.535131	-5.587197
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81	1	0	7.567152	-9.122453	-7.049362
82	1	0	8.574518	-9.987746	-5.902142
83	1	0	5.403758	-12.112334	-7.916349
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85	1	0	7.837687	-11.495525	-7.767046
86	1	0	7.216418	-12.055255	-6.222350
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88	7	0	-8.410230	-6.904723	4.606318
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91	6	0	-5.866870	2.733796	0.438343
92	6	0	-6.503413	0.264227	1.540687
93	6	0	-4.944805	2.043181	1.174733
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164	1	0	-10.971183	-6.677817	4.167170
165	1	0	-9.030988	-5.973813	6.408743
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40	6	0	-5.613433	8.322756	-2.113403
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42	6	0	-8.322756	5.613433	2.113403
43	6	0	-8.044421	5.868363	3.431322
44	6	0	-6.345009	7.475831	2.727723
45	6	0	-7.015359	6.820802	3.718609
46	6	0	-4.970460	9.000679	0.650033
47	6	0	-3.589906	8.781180	0.544122
48	6	0	-5.407937	10.259463	1.072804
49	6	0	-2.680524	9.789879	0.845940
50	6	0	-4.494550	11.266434	1.378671
51	6	0	-3.120229	11.047734	1.272710
52	6	0	-2.131974	12.150523	1.577439
53	1	0	-8.191418	5.574893	-2.984813
54	1	0	-7.033985	6.757489	-4.749631
55	1	0	-4.901317	9.090773	-1.851401
56	6	0	-5.185836	8.780372	-4.594145
57	1	0	-9.090773	4.901317	1.851401
58	6	0	-8.780372	5.185836	4.594145

59	1	0	-5.574893	8.191418	2.984813
60	1	0	-6.757489	7.033985	4.749631
61	1	0	-3.231550	7.809359	0.222486
62	1	0	-6.471995	10.450652	1.157712
63	1	0	-1.615656	9.610254	0.746667
64	1	0	-4.857595	12.236704	1.703671
65	6	0	-0.574109	13.752008	0.519001
66	6	0	0.574109	13.752008	-0.519001
67	6	0	-1.392447	15.062007	0.443805
68	6	0	1.392447	15.062007	-0.443805
69	6	0	-0.543981	16.334400	0.539004
70	6	0	0.543981	16.334400	-0.539004
71	7	0	-1.420899	12.564011	0.363953
72	7	0	1.420899	12.564011	-0.363953
73	1	0	-0.109249	13.684376	1.512101
74	1	0	0.109249	13.684376	-1.512101
75	1	0	-1.929887	15.067238	-0.515228
76	1	0	-2.157880	15.055209	1.226009
77	1	0	1.929887	15.067238	0.515228
78	1	0	2.157880	15.055209	-1.226009
79	1	0	-1.181311	17.219803	0.445837
80	1	0	-0.074811	16.391654	1.529676
81	1	0	1.181311	17.219803	-0.445837
82	1	0	0.074811	16.391654	-1.529676
83	1	0	-1.382577	11.789382	2.291734
84	6	0	-2.131974	-12.150523	-1.577439
85	6	0	-3.120229	-11.047734	-1.272710
86	1	0	-1.382577	-11.789382	-2.291734
87	6	0	-4.970460	-9.000679	-0.650033
88	6	0	-3.589906	-8.781180	-0.544122
89	6	0	-5.407937	-10.259463	-1.072804
90	6	0	-2.680524	-9.789879	-0.845940
91	6	0	-4.494550	-11.266434	-1.378671
92	1	0	-3.231550	-7.809359	-0.222486
93	1	0	-6.471995	-10.450652	-1.157712
94	1	0	-1.615656	-9.610254	-0.746667
95	1	0	-4.857595	-12.236704	-1.703671
96	6	0	-5.962084	-7.931713	-0.313967
97	6	0	-6.256380	-7.634455	1.033295
98	6	0	-6.628820	-7.240155	-1.345439
99	6	0	-7.240155	-6.628820	1.345439
100	6	0	-7.634455	-6.256380	-1.033295
101	6	0	-7.931713	-5.962084	0.313967
102	6	0	-5.613433	-8.322756	2.113403
103	6	0	-5.868363	-8.044421	3.431322
104	6	0	-7.475831	-6.345009	2.727723
105	6	0	-6.820802	-7.015359	3.718609
106	6	0	-6.345009	-7.475831	-2.727723
107	6	0	-7.015359	-6.820802	-3.718609
108	6	0	-8.322756	-5.613433	-2.113403
109	6	0	-8.044421	-5.868363	-3.431322
110	6	0	-9.000679	-4.970460	0.650033

	111	6	0	-10.259463	-5.407937	1.072804
	112	6	0	-8.781180	-3.589906	0.544122
	113	6	0	-11.266434	-4.494550	1.378671
	114	6	0	-9.789879	-2.680524	0.845940
	115	6	0	-11.047734	-3.120229	1.272710
	116	1	0	-4.901317	-9.090773	1.851401
	117	6	0	-5.185836	-8.780372	4.594145
	118	1	0	-8.191418	-5.574893	2.984813
	119	1	0	-7.033985	-6.757489	4.749631
	120	1	0	-5.574893	-8.191418	-2.984813
	121	1	0	-6.757489	-7.033985	-4.749631
	122	1	0	-9.090773	-4.901317	-1.851401
	123	6	0	-8.780372	-5.185836	-4.594145
	124	1	0	-10.450652	-6.471995	1.157712
	125	1	0	-7.809359	-3.231550	0.222486
	126	1	0	-12.236704	-4.857595	1.703671
	127	1	0	-9.610254	-1.615656	0.746667
	128	1	0	-11.789382	-1.382577	2.291734
	129	6	0	-4.413207	7.761430	-5.464753
	130	6	0	-4.189727	9.848364	-4.109097
	131	6	0	-6.261081	9.480294	-5.458437
	132	6	0	-9.480294	6.261081	5.458437
	133	6	0	-7.761430	4.413207	5.464753
	134	6	0	-9.480294	-6.261081	-5.458437
	135	6	0	-7.761430	-4.413207	-5.464753
	136	6	0	-9.848364	-4.189727	-4.109097
	137	6	0	-4.413207	-7.761430	5.464753
	138	6	0	-6.261081	-9.480294	5.458437
	139	6	0	-4.189727	-9.848364	4.109097
	140	1	0	-5.071976	6.995051	-5.879363
	141	1	0	-3.640471	7.256739	-4.878694
	142	1	0	-3.926991	8.270433	-6.302755
	143	1	0	-3.385344	9.412292	-3.510950
	144	1	0	-4.681327	10.618569	-3.508820
	145	1	0	-3.731653	10.341709	-4.970697
	146	1	0	-6.814626	10.216420	-4.869100
	147	1	0	-6.982929	8.769713	-5.867917
	148	1	0	-5.792141	10.000261	-6.299622
	149	1	0	-10.216420	6.814626	4.869100
	150	1	0	-8.769713	6.982929	5.867917
	151	1	0	-10.000261	5.792141	6.299622
	152	1	0	-6.995051	5.071976	5.879363
	153	1	0	-7.256739	3.640471	4.878694
	154	1	0	-8.270433	3.926991	6.302755
	155	1	0	-10.216420	-6.814626	-4.869100
	156	1	0	-8.769713	-6.982929	-5.867917
	157	1	0	-10.000261	-5.792141	-6.299622
	158	1	0	-6.995051	-5.071976	-5.879363
	159	1	0	-7.256739	-3.640471	-4.878694
	160	1	0	-8.270433	-3.926991	-6.302755
	161	1	0	-9.412292	-3.385344	-3.510950
	162	1	0	-10.618569	-4.681327	-3.508820

	163	1	0	-10.341709	-3.731653	-4.970697
	164	1	0	-5.071976	-6.995051	5.879363
	165	1	0	-3.640471	-7.256739	4.878694
	166	1	0	-3.926991	-8.270433	6.302755
	167	1	0	-6.814626	-10.216420	4.869100
	168	1	0	-6.982929	-8.769713	5.867917
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	170	1	0	-3.385344	-9.412292	3.510950
	171	1	0	-4.681327	-10.618569	3.508820
	172	1	0	-3.731653	-10.341709	4.970697
	173	6	0	-9.848364	4.189727	4.109097
	174	1	0	-9.412292	3.385344	3.510950
	175	1	0	-10.618569	4.681327	3.508820
	176	1	0	-10.341709	3.731653	4.970697
	177	1	0	-12.973675	-2.671174	2.076139
	178	1	0	-12.973675	2.671174	-2.076139
	179	1	0	-2.671174	12.973675	2.076139
	180	1	0	-2.671174	-12.973675	-2.076139
	181	6	0	13.752008	0.574109	0.519001
	182	6	0	13.752008	-0.574109	-0.519001
	183	6	0	15.062007	1.392447	0.443805
	184	6	0	15.062007	-1.392447	-0.443805
	185	6	0	16.334400	0.543981	0.539004
	186	6	0	16.334400	-0.543981	-0.539004
	187	7	0	12.564011	1.420899	0.363953
	188	7	0	12.564011	-1.420899	-0.363953
	189	6	0	12.150523	2.131974	1.577439
	190	6	0	12.150523	-2.131974	-1.577439
	191	6	0	11.047734	-3.120229	-1.272710
	192	1	0	13.684376	0.109249	1.512101
	193	1	0	13.684376	-0.109249	-1.512101
	194	1	0	11.789382	-1.382577	-2.291734
	195	1	0	15.067238	1.929887	-0.515228
	196	1	0	15.055209	2.157880	1.226009
	197	1	0	15.067238	-1.929887	0.515228
	198	1	0	15.055209	-2.157880	-1.226009
	199	1	0	17.219803	1.181311	0.445837
	200	1	0	16.391654	0.074811	1.529676
	201	1	0	17.219803	-1.181311	-0.445837
	202	1	0	16.391654	-0.074811	-1.529676
	203	6	0	9.000679	-4.970460	-0.650033
	204	6	0	10.259463	-5.407937	-1.072804
	205	6	0	8.781180	-3.589906	-0.544122
	206	6	0	11.266434	-4.494550	-1.378671
	207	6	0	9.789879	-2.680524	-0.845940
	208	1	0	10.450652	-6.471995	-1.157712
	209	1	0	7.809359	-3.231550	-0.222486
	210	1	0	12.236704	-4.857595	-1.703671
	211	1	0	9.610254	-1.615656	-0.746667
	212	6	0	7.931713	-5.962084	-0.313967
	213	6	0	7.240155	-6.628820	-1.345439
	214	6	0	7.634455	-6.256380	1.033295

215	6	0	6.256380	-7.634455	-1.033295
216	6	0	6.628820	-7.240155	1.345439
217	6	0	5.962084	-7.931713	0.313967
218	6	0	7.475831	-6.345009	-2.727723
219	6	0	6.820802	-7.015359	-3.718609
220	6	0	5.613433	-8.322756	-2.113403
221	6	0	5.868363	-8.044421	-3.431322
222	6	0	8.322756	-5.613433	2.113403
223	6	0	8.044421	-5.868363	3.431322
224	6	0	6.345009	-7.475831	2.727723
225	6	0	7.015359	-6.820802	3.718609
226	6	0	4.970460	-9.000679	0.650033
227	6	0	3.589906	-8.781180	0.544122
228	6	0	5.407937	-10.259463	1.072804
229	6	0	2.680524	-9.789879	0.845940
230	6	0	4.494550	-11.266434	1.378671
231	6	0	3.120229	-11.047734	1.272710
232	6	0	2.131974	-12.150523	1.577439
233	1	0	8.191418	-5.574893	-2.984813
234	1	0	7.033985	-6.757489	-4.749631
235	1	0	4.901317	-9.090773	-1.851401
236	6	0	5.185836	-8.780372	-4.594145
237	1	0	9.090773	-4.901317	1.851401
238	6	0	8.780372	-5.185836	4.594145
239	1	0	5.574893	-8.191418	2.984813
240	1	0	6.757489	-7.033985	4.749631
241	1	0	3.231550	-7.809359	0.222486
242	1	0	6.471995	-10.450652	1.157712
243	1	0	1.615656	-9.610254	0.746667
244	1	0	4.857595	-12.236704	1.703671
245	6	0	0.574109	-13.752008	0.519001
246	6	0	-0.574109	-13.752008	-0.519001
247	6	0	1.392447	-15.062007	0.443805
248	6	0	-1.392447	-15.062007	-0.443805
249	6	0	0.543981	-16.334400	0.539004
250	6	0	-0.543981	-16.334400	-0.539004
251	7	0	1.420899	-12.564011	0.363953
252	7	0	-1.420899	-12.564011	-0.363953
253	1	0	0.109249	-13.684376	1.512101
254	1	0	-0.109249	-13.684376	-1.512101
255	1	0	1.929887	-15.067238	-0.515228
256	1	0	2.157880	-15.055209	1.226009
257	1	0	-1.929887	-15.067238	0.515228
258	1	0	-2.157880	-15.055209	-1.226009
259	1	0	1.181311	-17.219803	0.445837
260	1	0	0.074811	-16.391654	1.529676
261	1	0	-1.181311	-17.219803	-0.445837
262	1	0	-0.074811	-16.391654	-1.529676
263	1	0	1.382577	-11.789382	2.291734
264	6	0	2.131974	12.150523	-1.577439
265	6	0	3.120229	11.047734	-1.272710
266	1	0	1.382577	11.789382	-2.291734

267	6	0	4.970460	9.000679	-0.650033
268	6	0	3.589906	8.781180	-0.544122
269	6	0	5.407937	10.259463	-1.072804
270	6	0	2.680524	9.789879	-0.845940
271	6	0	4.494550	11.266434	-1.378671
272	1	0	3.231550	7.809359	-0.222486
273	1	0	6.471995	10.450652	-1.157712
274	1	0	1.615656	9.610254	-0.746667
275	1	0	4.857595	12.236704	-1.703671
276	6	0	5.962084	7.931713	-0.313967
277	6	0	6.256380	7.634455	1.033295
278	6	0	6.628820	7.240155	-1.345439
279	6	0	7.240155	6.628820	1.345439
280	6	0	7.634455	6.256380	-1.033295
281	6	0	7.931713	5.962084	0.313967
282	6	0	5.613433	8.322756	2.113403
283	6	0	5.868363	8.044421	3.431322
284	6	0	7.475831	6.345009	2.727723
285	6	0	6.820802	7.015359	3.718609
286	6	0	6.345009	7.475831	-2.727723
287	6	0	7.015359	6.820802	-3.718609
288	6	0	8.322756	5.613433	-2.113403
289	6	0	8.044421	5.868363	-3.431322
290	6	0	9.000679	4.970460	0.650033
291	6	0	10.259463	5.407937	1.072804
292	6	0	8.781180	3.589906	0.544122
293	6	0	11.266434	4.494550	1.378671
294	6	0	9.789879	2.680524	0.845940
295	6	0	11.047734	3.120229	1.272710
296	1	0	4.901317	9.090773	1.851401
297	6	0	5.185836	8.780372	4.594145
298	1	0	8.191418	5.574893	2.984813
299	1	0	7.033985	6.757489	4.749631
300	1	0	5.574893	8.191418	-2.984813
301	1	0	6.757489	7.033985	-4.749631
302	1	0	9.090773	4.901317	-1.851401
303	6	0	8.780372	5.185836	-4.594145
304	1	0	10.450652	6.471995	1.157712
305	1	0	7.809359	3.231550	0.222486
306	1	0	12.236704	4.857595	1.703671
307	1	0	9.610254	1.615656	0.746667
308	1	0	11.789382	1.382577	2.291734
309	6	0	4.413207	-7.761430	-5.464753
310	6	0	4.189727	-9.848364	-4.109097
311	6	0	6.261081	-9.480294	-5.458437
312	6	0	9.480294	-6.261081	5.458437
313	6	0	7.761430	-4.413207	5.464753
314	6	0	9.480294	6.261081	-5.458437
315	6	0	7.761430	4.413207	-5.464753
316	6	0	9.848364	4.189727	-4.109097
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	319	6	0	4.189727	9.848364	4.109097
	320	1	0	5.071976	-6.995051	-5.879363
	321	1	0	3.640471	-7.256739	-4.878694
	322	1	0	3.926991	-8.270433	-6.302755
	323	1	0	3.385344	-9.412292	-3.510950
	324	1	0	4.681327	-10.618569	-3.508820
	325	1	0	3.731653	-10.341709	-4.970697
	326	1	0	6.814626	-10.216420	-4.869100
	327	1	0	6.982929	-8.769713	-5.867917
	328	1	0	5.792141	-10.000261	-6.299622
	329	1	0	10.216420	-6.814626	4.869100
	330	1	0	8.769713	-6.982929	5.867917
	331	1	0	10.000261	-5.792141	6.299622
	332	1	0	6.995051	-5.071976	5.879363
	333	1	0	7.256739	-3.640471	4.878694
	334	1	0	8.270433	-3.926991	6.302755
	335	1	0	10.216420	6.814626	-4.869100
	336	1	0	8.769713	6.982929	-5.867917
	337	1	0	10.000261	5.792141	-6.299622
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	340	1	0	8.270433	3.926991	-6.302755
	341	1	0	9.412292	3.385344	-3.510950
	342	1	0	10.618569	4.681327	-3.508820
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	355	1	0	10.618569	-4.681327	3.508820
	356	1	0	10.341709	-3.731653	4.970697
	357	1	0	12.973675	2.671174	2.076139
	358	1	0	12.973675	-2.671174	-2.076139
	359	1	0	2.671174	-12.973675	2.076139
	360	1	0	2.671174	12.973675	-2.076139
	361	1	0	2.096786	12.723811	0.377998
	362	1	0	-2.096786	12.723811	-0.377998
	363	1	0	12.723811	-2.096786	0.377998
	364	1	0	12.723811	2.096786	-0.377998
	365	1	0	2.096786	-12.723811	-0.377998
	366	1	0	-2.096786	-12.723811	0.377998
	367	1	0	-12.723811	2.096786	0.377998
	368	1	0	-12.723811	-2.096786	-0.377998
5 (C_4)	1	6	0	-4.197503	13.278172	0.180634
	2	6	0	-5.327679	12.747723	-0.718098

	3	6	0	-3.962180	14.745894	-0.117459
	4	6	0	-6.563838	13.647634	-0.625227
	5	6	0	-5.211384	15.599053	0.112520
	6	6	0	-6.298778	15.126164	-0.833456
	7	7	0	-2.999331	12.485442	-0.040996
	8	7	0	-5.589660	11.327104	-0.411454
	9	6	0	-2.081150	12.544668	1.084465
	10	6	0	-6.517613	10.722818	-1.367708
	11	6	0	-6.959060	9.341223	-0.987819
	12	1	0	-4.551115	13.186561	1.235306
	13	1	0	-4.884081	12.746420	-1.727123
	14	1	0	-5.974164	10.709086	-2.325089
	15	1	0	-3.615941	14.841690	-1.154407
	16	1	0	-3.123979	15.114593	0.490888
	17	1	0	-7.023874	13.486704	0.361292
	18	1	0	-7.321612	13.314641	-1.342398
	19	1	0	-4.977894	16.664341	0.002729
	20	1	0	-5.554107	15.492362	1.151499
	21	1	0	-7.225083	15.703759	-0.716847
	22	1	0	-5.964154	15.285145	-1.868846
	23	6	0	-7.777575	6.700816	-0.364783
	24	6	0	-8.616924	7.584287	-1.063164
	25	6	0	-6.513034	7.165962	0.000081
	26	6	0	-8.226690	8.879608	-1.341679
	27	6	0	-6.109647	8.462105	-0.311483
	28	1	0	-9.607276	7.225931	-1.331716
	29	1	0	-5.837372	6.486045	0.511410
	30	1	0	-8.894743	9.551959	-1.875175
	31	1	0	-5.116643	8.800798	-0.020985
	32	6	0	-8.339876	5.360841	-0.080568
	33	6	0	-7.951369	4.267751	-0.886179
	34	6	0	-9.358698	5.206204	0.874445
	35	6	0	-8.631103	2.999329	-0.782607
	36	6	0	-10.083888	3.973198	0.909654
	37	6	0	-9.732842	2.878715	0.082745
	38	6	0	-6.867405	4.343817	-1.808332
	39	6	0	-6.470362	3.249627	-2.517154
	40	6	0	-8.176864	1.881272	-1.552649
	41	6	0	-7.095520	1.969731	-2.384365
	42	6	0	-9.709323	6.242001	1.785606
	43	6	0	-10.754992	6.132752	2.664957
	44	6	0	-11.223112	3.913476	1.766553
	45	6	0	-11.518988	4.925394	2.637272
	46	6	0	-10.420922	1.581938	0.290876
	47	6	0	-10.083204	0.806293	1.397229
	48	6	0	-11.419791	1.121431	-0.577567
	49	6	0	-10.754992	-0.376360	1.687138
	50	6	0	-12.069748	-0.068170	-0.303135
	51	6	0	-11.757563	-0.826493	0.835699
	52	6	0	-12.544668	-2.081150	1.084465
	53	1	0	-6.335107	5.281225	-1.931733
	54	1	0	-5.589820	3.319241	-3.152759

55	1	0	-8.719327	0.964794	-1.353818
56	6	0	-6.485188	0.799451	-3.135635
57	1	0	-9.064141	7.116840	1.813770
58	6	0	-11.101195	7.211170	3.688621
59	1	0	-11.823063	3.012575	1.778275
60	1	0	-12.348410	4.759633	3.316221
61	1	0	-9.306408	1.183421	2.062387
62	1	0	-11.685359	1.729619	-1.437720
63	1	0	-10.487227	-0.962370	2.559918
64	1	0	-12.850921	-0.473483	-0.944939
65	6	0	-13.278172	-4.197503	0.180634
66	6	0	-12.747723	-5.327679	-0.718098
67	6	0	-14.745894	-3.962180	-0.117459
68	6	0	-13.647634	-6.563838	-0.625227
69	6	0	-15.599053	-5.211384	0.112520
70	6	0	-15.126164	-6.298778	-0.833456
71	7	0	-12.485442	-2.999331	-0.040996
72	7	0	-11.327104	-5.589660	-0.411454
73	1	0	-13.186561	-4.551115	1.235306
74	1	0	-12.746420	-4.884081	-1.727123
75	1	0	-14.841690	-3.615941	-1.154407
76	1	0	-15.114593	-3.123979	0.490888
77	1	0	-13.486704	-7.023874	0.361292
78	1	0	-13.314641	-7.321612	-1.342398
79	1	0	-16.664341	-4.977894	0.002729
80	1	0	-15.492362	-5.554107	1.151499
81	1	0	-15.703759	-7.225083	-0.716847
82	1	0	-15.285145	-5.964154	-1.868846
83	1	0	-12.183665	-2.546551	2.022837
84	6	0	10.722818	6.517613	-1.367708
85	6	0	9.341223	6.959060	-0.987819
86	1	0	10.709086	5.974164	-2.325089
87	6	0	6.700816	7.777575	-0.364783
88	6	0	7.165962	6.513034	0.000081
89	6	0	7.584287	8.616924	-1.063164
90	6	0	8.462105	6.109647	-0.311483
91	6	0	8.879608	8.226690	-1.341679
92	1	0	6.486045	5.837372	0.511410
93	1	0	7.225931	9.607276	-1.331716
94	1	0	8.800798	5.116643	-0.020985
95	1	0	9.551959	8.894743	-1.875175
96	6	0	5.360841	8.339876	-0.080568
97	6	0	5.206204	9.358698	0.874445
98	6	0	4.267751	7.951369	-0.886179
99	6	0	3.973198	10.083888	0.909654
100	6	0	2.999329	8.631103	-0.782607
101	6	0	2.878715	9.732842	0.082745
102	6	0	6.242001	9.709323	1.785606
103	6	0	6.132752	10.754992	2.664957
104	6	0	3.913476	11.223112	1.766553
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	107	6	0	3.249627	6.470362	-2.517154
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	109	6	0	1.969731	7.095520	-2.384365
	110	6	0	1.581938	10.420922	0.290876
	111	6	0	1.121431	11.419791	-0.577567
	112	6	0	0.806293	10.083204	1.397229
	113	6	0	-0.068170	12.069748	-0.303135
	114	6	0	-0.376360	10.754992	1.687138
	115	6	0	-0.826493	11.757563	0.835699
	116	1	0	7.116840	9.064141	1.813770
	117	6	0	7.211170	11.101195	3.688621
	118	1	0	3.012575	11.823063	1.778275
	119	1	0	4.759633	12.348410	3.316221
	120	1	0	5.281225	6.335107	-1.931733
	121	1	0	3.319241	5.589820	-3.152759
	122	1	0	0.964794	8.719327	-1.353818
	123	6	0	0.799451	6.485188	-3.135635
	124	1	0	1.729619	11.685359	-1.437720
	125	1	0	1.183421	9.306408	2.062387
	126	1	0	-0.473483	12.850921	-0.944939
	127	1	0	-0.962370	10.487227	2.559918
	128	1	0	-2.546551	12.183665	2.022837
	129	6	0	-5.046007	0.530951	-2.684729
	130	6	0	-7.310360	-0.472778	-2.862783
	131	6	0	-6.549937	1.120802	-4.639668
	132	6	0	-12.564666	7.597316	3.446715
	133	6	0	-10.953553	6.626831	5.103710
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	137	6	0	6.626831	10.953553	5.103710
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	140	1	0	-4.406429	1.416778	-2.758275
	141	1	0	-5.015051	0.187088	-1.649847
	142	1	0	-4.612439	-0.256211	-3.309940
	143	1	0	-7.326508	-0.715986	-1.798260
	144	1	0	-8.349471	-0.351907	-3.186896
	145	1	0	-6.883080	-1.332128	-3.387015
	146	1	0	-7.569601	1.327023	-4.970774
	147	1	0	-5.955058	2.005858	-4.881057
	148	1	0	-6.180851	0.289621	-5.249560
	149	1	0	-12.693983	8.059142	2.465475
	150	1	0	-13.233911	6.738673	3.492606
	151	1	0	-12.919292	8.319357	4.191373
	152	1	0	-11.526841	5.708364	5.231212
	153	1	0	-9.903867	6.407270	5.313015
	154	1	0	-11.291285	7.344217	5.856665
	155	1	0	1.327023	7.569601	-4.970774
	156	1	0	2.005858	5.955058	-4.881057
	157	1	0	0.289621	6.180851	-5.249560
	158	1	0	1.416778	4.406429	-2.758275

159	1	0	0.187088	5.015051	-1.649847
160	1	0	-0.256211	4.612439	-3.309940
161	1	0	-0.715986	7.326508	-1.798260
162	1	0	-0.351907	8.349471	-3.186896
163	1	0	-1.332128	6.883080	-3.387015
164	1	0	5.708364	11.526841	5.231212
165	1	0	6.407270	9.903867	5.313015
166	1	0	7.344217	11.291285	5.856665
167	1	0	8.059142	12.693983	2.465475
168	1	0	6.738673	13.233911	3.492606
169	1	0	8.319357	12.919292	4.191373
170	1	0	8.247386	9.179034	3.688690
171	1	0	8.960622	10.379814	2.595332
172	1	0	9.183170	10.514327	4.346155
173	6	0	-10.241627	8.465393	3.566686
174	1	0	-9.179034	8.247386	3.688690
175	1	0	-10.379814	8.960622	2.595332
176	1	0	-10.514327	9.183170	4.346155
177	1	0	-3.283750	11.519695	-0.190984
178	1	0	-1.810409	13.593548	1.266489
179	1	0	-7.444936	11.290434	-1.569493
180	1	0	-13.593548	-1.810409	1.266489
181	1	0	-11.519695	-3.283750	-0.190984
182	1	0	11.290434	7.444936	-1.569493
183	6	0	4.197503	-13.278172	0.180634
184	6	0	5.327679	-12.747723	-0.718098
185	6	0	3.962180	-14.745894	-0.117459
186	6	0	6.563838	-13.647634	-0.625227
187	6	0	5.211384	-15.599053	0.112520
188	6	0	6.298778	-15.126164	-0.833456
189	7	0	2.999331	-12.485442	-0.040996
190	7	0	5.589660	-11.327104	-0.411454
191	6	0	2.081150	-12.544668	1.084465
192	6	0	6.517613	-10.722818	-1.367708
193	6	0	6.959060	-9.341223	-0.987819
194	1	0	4.551115	-13.186561	1.235306
195	1	0	4.884081	-12.746420	-1.727123
196	1	0	5.974164	-10.709086	-2.325089
197	1	0	3.615941	-14.841690	-1.154407
198	1	0	3.123979	-15.114593	0.490888
199	1	0	7.023874	-13.486704	0.361292
200	1	0	7.321612	-13.314641	-1.342398
201	1	0	4.977894	-16.664341	0.002729
202	1	0	5.554107	-15.492362	1.151499
203	1	0	7.225083	-15.703759	-0.716847
204	1	0	5.964154	-15.285145	-1.868846
205	6	0	7.777575	-6.700816	-0.364783
206	6	0	8.616924	-7.584287	-1.063164
207	6	0	6.513034	-7.165962	0.000081
208	6	0	8.226690	-8.879608	-1.341679
209	6	0	6.109647	-8.462105	-0.311483
210	1	0	9.607276	-7.225931	-1.331716

	211	1	0	5.837372	-6.486045	0.511410
	212	1	0	8.894743	-9.551959	-1.875175
	213	1	0	5.116643	-8.800798	-0.020985
	214	6	0	8.339876	-5.360841	-0.080568
	215	6	0	7.951369	-4.267751	-0.886179
	216	6	0	9.358698	-5.206204	0.874445
	217	6	0	8.631103	-2.999329	-0.782607
	218	6	0	10.083888	-3.973198	0.909654
	219	6	0	9.732842	-2.878715	0.082745
	220	6	0	6.867405	-4.343817	-1.808332
	221	6	0	6.470362	-3.249627	-2.517154
	222	6	0	8.176864	-1.881272	-1.552649
	223	6	0	7.095520	-1.969731	-2.384365
	224	6	0	9.709323	-6.242001	1.785606
	225	6	0	10.754992	-6.132752	2.664957
	226	6	0	11.223112	-3.913476	1.766553
	227	6	0	11.518988	-4.925394	2.637272
	228	6	0	10.420922	-1.581938	0.290876
	229	6	0	10.083204	-0.806293	1.397229
	230	6	0	11.419791	-1.121431	-0.577567
	231	6	0	10.754992	0.376360	1.687138
	232	6	0	12.069748	0.068170	-0.303135
	233	6	0	11.757563	0.826493	0.835699
	234	6	0	12.544668	2.081150	1.084465
	235	1	0	6.335107	-5.281225	-1.931733
	236	1	0	5.589820	-3.319241	-3.152759
	237	1	0	8.719327	-0.964794	-1.353818
	238	6	0	6.485188	-0.799451	-3.135635
	239	1	0	9.064141	-7.116840	1.813770
	240	6	0	11.101195	-7.211170	3.688621
	241	1	0	11.823063	-3.012575	1.778275
	242	1	0	12.348410	-4.759633	3.316221
	243	1	0	9.306408	-1.183421	2.062387
	244	1	0	11.685359	-1.729619	-1.437720
	245	1	0	10.487227	0.962370	2.559918
	246	1	0	12.850921	0.473483	-0.944939
	247	6	0	13.278172	4.197503	0.180634
	248	6	0	12.747723	5.327679	-0.718098
	249	6	0	14.745894	3.962180	-0.117459
	250	6	0	13.647634	6.563838	-0.625227
	251	6	0	15.599053	5.211384	0.112520
	252	6	0	15.126164	6.298778	-0.833456
	253	7	0	12.485442	2.999331	-0.040996
	254	7	0	11.327104	5.589660	-0.411454
	255	1	0	13.186561	4.551115	1.235306
	256	1	0	12.746420	4.884081	-1.727123
	257	1	0	14.841690	3.615941	-1.154407
	258	1	0	15.114593	3.123979	0.490888
	259	1	0	13.486704	7.023874	0.361292
	260	1	0	13.314641	7.321612	-1.342398
	261	1	0	16.664341	4.977894	0.002729
	262	1	0	15.492362	5.554107	1.151499

263	1	0	15.703759	7.225083	-0.716847
264	1	0	15.285145	5.964154	-1.868846
265	1	0	12.183665	2.546551	2.022837
266	6	0	-10.722818	-6.517613	-1.367708
267	6	0	-9.341223	-6.959060	-0.987819
268	1	0	-10.709086	-5.974164	-2.325089
269	6	0	-6.700816	-7.777575	-0.364783
270	6	0	-7.165962	-6.513034	0.000081
271	6	0	-7.584287	-8.616924	-1.063164
272	6	0	-8.462105	-6.109647	-0.311483
273	6	0	-8.879608	-8.226690	-1.341679
274	1	0	-6.486045	-5.837372	0.511410
275	1	0	-7.225931	-9.607276	-1.331716
276	1	0	-8.800798	-5.116643	-0.020985
277	1	0	-9.551959	-8.894743	-1.875175
278	6	0	-5.360841	-8.339876	-0.080568
279	6	0	-5.206204	-9.358698	0.874445
280	6	0	-4.267751	-7.951369	-0.886179
281	6	0	-3.973198	-10.083888	0.909654
282	6	0	-2.999329	-8.631103	-0.782607
283	6	0	-2.878715	-9.732842	0.082745
284	6	0	-6.242001	-9.709323	1.785606
285	6	0	-6.132752	-10.754992	2.664957
286	6	0	-3.913476	-11.223112	1.766553
287	6	0	-4.925394	-11.518988	2.637272
288	6	0	-4.343817	-6.867405	-1.808332
289	6	0	-3.249627	-6.470362	-2.517154
290	6	0	-1.881272	-8.176864	-1.552649
291	6	0	-1.969731	-7.095520	-2.384365
292	6	0	-1.581938	-10.420922	0.290876
293	6	0	-1.121431	-11.419791	-0.577567
294	6	0	-0.806293	-10.083204	1.397229
295	6	0	0.068170	-12.069748	-0.303135
296	6	0	0.376360	-10.754992	1.687138
297	6	0	0.826493	-11.757563	0.835699
298	1	0	-7.116840	-9.064141	1.813770
299	6	0	-7.211170	-11.101195	3.688621
300	1	0	-3.012575	-11.823063	1.778275
301	1	0	-4.759633	-12.348410	3.316221
302	1	0	-5.281225	-6.335107	-1.931733
303	1	0	-3.319241	-5.589820	-3.152759
304	1	0	-0.964794	-8.719327	-1.353818
305	6	0	-0.799451	-6.485188	-3.135635
306	1	0	-1.729619	-11.685359	-1.437720
307	1	0	-1.183421	-9.306408	2.062387
308	1	0	0.473483	-12.850921	-0.944939
309	1	0	0.962370	-10.487227	2.559918
310	1	0	2.546551	-12.183665	2.022837
311	6	0	5.046007	-0.530951	-2.684729
312	6	0	7.310360	0.472778	-2.862783
313	6	0	6.549937	-1.120802	-4.639668
314	6	0	12.564666	-7.597316	3.446715

	315	6	0	10.953553	-6.626831	5.103710
	316	6	0	-1.120802	-6.549937	-4.639668
	317	6	0	-0.530951	-5.046007	-2.684729
	318	6	0	0.472778	-7.310360	-2.862783
	319	6	0	-6.626831	-10.953553	5.103710
	320	6	0	-7.597316	-12.564666	3.446715
	321	6	0	-8.465393	-10.241627	3.566686
	322	1	0	4.406429	-1.416778	-2.758275
	323	1	0	5.015051	-0.187088	-1.649847
	324	1	0	4.612439	0.256211	-3.309940
	325	1	0	7.326508	0.715986	-1.798260
	326	1	0	8.349471	0.351907	-3.186896
	327	1	0	6.883080	1.332128	-3.387015
	328	1	0	7.569601	-1.327023	-4.970774
	329	1	0	5.955058	-2.005858	-4.881057
	330	1	0	6.180851	-0.289621	-5.249560
	331	1	0	12.693983	-8.059142	2.465475
	332	1	0	13.233911	-6.738673	3.492606
	333	1	0	12.919292	-8.319357	4.191373
	334	1	0	11.526841	-5.708364	5.231212
	335	1	0	9.903867	-6.407270	5.313015
	336	1	0	11.291285	-7.344217	5.856665
	337	1	0	-1.327023	-7.569601	-4.970774
	338	1	0	-2.005858	-5.955058	-4.881057
	339	1	0	-0.289621	-6.180851	-5.249560
	340	1	0	-1.416778	-4.406429	-2.758275
	341	1	0	-0.187088	-5.015051	-1.649847
	342	1	0	0.256211	-4.612439	-3.309940
	343	1	0	0.715986	-7.326508	-1.798260
	344	1	0	0.351907	-8.349471	-3.186896
	345	1	0	1.332128	-6.883080	-3.387015
	346	1	0	-5.708364	-11.526841	5.231212
	347	1	0	-6.407270	-9.903867	5.313015
	348	1	0	-7.344217	-11.291285	5.856665
	349	1	0	-8.059142	-12.693983	2.465475
	350	1	0	-6.738673	-13.233911	3.492606
	351	1	0	-8.319357	-12.919292	4.191373
	352	1	0	-8.247386	-9.179034	3.688690
	353	1	0	-8.960622	-10.379814	2.595332
	354	1	0	-9.183170	-10.514327	4.346155
	355	6	0	10.241627	-8.465393	3.566686
	356	1	0	9.179034	-8.247386	3.688690
	357	1	0	10.379814	-8.960622	2.595332
	358	1	0	10.514327	-9.183170	4.346155
	359	1	0	3.283750	-11.519695	-0.190984
	360	1	0	1.810409	-13.593548	1.266489
	361	1	0	7.444936	-11.290434	-1.569493
	362	1	0	13.593548	1.810409	1.266489
	363	1	0	11.519695	3.283750	-0.190984
	364	1	0	-11.290434	-7.444936	-1.569493
	365	1	0	-11.248134	-5.967181	0.533082
	366	1	0	5.967181	-11.248134	0.533082

	367	1	0	11.248134	5.967181	0.533082
	368	1	0	-5.967181	11.248134	0.533082
5×8H$^+$	1	6	0	10.450579	9.562207	-0.452988
	2	6	0	9.562207	10.450579	0.452988
	3	6	0	11.943801	9.909517	-0.266083
	4	6	0	9.909517	11.943801	0.266083
	5	6	0	12.248383	11.397987	-0.470534
	6	6	0	11.397987	12.248383	0.470534
	7	7	0	10.311867	8.051905	-0.172576
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	9	6	0	10.695679	7.109886	-1.362145
	10	6	0	7.109886	10.695679	1.362145
	11	6	0	5.664238	10.666070	0.968497
	12	1	0	10.161032	9.690159	-1.500182
	13	1	0	9.690159	10.161032	1.500182
	14	1	0	7.346593	9.977297	2.147839
	15	1	0	12.240136	9.623481	0.752511
	16	1	0	12.539017	9.308316	-0.956446
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	19	1	0	13.311416	11.564470	-0.288326
	20	1	0	12.066092	11.681109	-1.512885
	21	1	0	11.564470	13.311416	0.288326
	22	1	0	11.681109	12.066092	1.512885
	23	6	0	2.892788	10.659736	0.411747
	24	6	0	3.655872	11.827306	0.261016
	25	6	0	3.549009	9.489664	0.823927
	26	6	0	5.019801	11.834663	0.537821
	27	6	0	4.911314	9.490944	1.104269
	28	1	0	3.168793	12.746146	-0.042603
	29	1	0	2.975275	8.580250	0.956218
	30	1	0	5.568873	12.768164	0.458935
	31	1	0	5.375166	8.581643	1.477356
	32	6	0	1.409063	10.668442	0.190442
	33	6	0	0.546758	10.685812	1.307038
	34	6	0	0.884020	10.675877	-1.118818
	35	6	0	-0.884020	10.675877	1.118818
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	37	6	0	-1.409063	10.668442	-0.190442
	38	6	0	1.029140	10.743597	2.652042
	39	6	0	0.181268	10.769732	3.719432
	40	6	0	-1.727231	10.678027	2.276687
	41	6	0	-1.240007	10.729620	3.558196
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	44	6	0	-1.029140	10.743597	-2.652042
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53	1	0	2.096037	10.787628	2.827951
54	1	0	0.600790	10.830987	4.715777
55	1	0	-2.794855	10.650294	2.115272
56	6	0	-2.131605	10.762914	4.806780
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62	1	0	-3.168793	12.746146	0.042603
63	1	0	-5.375166	8.581643	-1.477356
64	1	0	-5.568873	12.768164	-0.458935
65	6	0	-9.562207	10.450579	-0.452988
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76	1	0	-9.308316	12.539017	-0.956446
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83	1	0	-7.346593	9.977297	-2.147839
84	6	0	10.695679	-7.109886	1.362145
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89	6	0	11.827306	-3.655872	0.261016
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92	1	0	8.580250	-2.975275	0.956218
93	1	0	12.746146	-3.168793	-0.042603
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96	6	0	10.668442	-1.409063	0.190442
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98	6	0	10.685812	-0.546758	1.307038
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103	6	0	10.729620	-1.240007	-3.558196
104	6	0	10.743597	1.029140	-2.652042
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112	6	0	9.489664	3.549009	-0.823927
113	6	0	11.834663	5.019801	-0.537821
114	6	0	9.490944	4.911314	-1.104269
115	6	0	10.666070	5.664238	-0.968497
116	1	0	10.650294	-2.794855	-2.115272
117	6	0	10.762914	-2.131605	-4.806780
118	1	0	10.787628	2.096037	-2.827951
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122	1	0	10.650294	2.794855	2.115272
123	6	0	10.762914	2.131605	4.806780
124	1	0	12.746146	3.168793	0.042603
125	1	0	8.580250	2.975275	-0.956218
126	1	0	12.768164	5.568873	-0.458935
127	1	0	8.581643	5.375166	-1.477356
128	1	0	9.977297	7.346593	-2.147839
129	6	0	-1.801218	9.547203	5.705036
130	6	0	-3.629931	10.710067	4.457894
131	6	0	-1.863167	12.071075	5.589205
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143	1	0	-3.889242	9.788921	3.925492
144	1	0	-3.934060	11.566154	3.848346
145	1	0	-4.217508	10.737903	5.378308
146	1	0	-2.087744	12.949264	4.978518
147	1	0	-0.824474	12.148320	5.916318
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	155	1	0	12.949264	2.087744	4.978518
	156	1	0	12.148320	0.824474	5.916318
	157	1	0	12.110368	2.490388	6.483386
	158	1	0	9.549668	0.759357	6.031740
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	160	1	0	9.563379	2.423802	6.603335
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	168	1	0	12.148320	-0.824474	-5.916318
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	170	1	0	9.788921	-3.889242	-3.925492
	171	1	0	11.566154	-3.934060	-3.848346
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	176	1	0	4.217508	10.737903	-5.378308
	177	1	0	9.374084	7.770299	0.122150
	178	1	0	7.770299	9.374084	-0.122150
	179	1	0	11.686532	7.431290	-1.676214
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	185	6	0	-10.450579	-9.562207	-0.452988
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	187	6	0	-11.943801	-9.909517	-0.266083
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	189	6	0	-12.248383	-11.397987	-0.470534
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	191	7	0	-10.311867	-8.051905	-0.172576
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	193	6	0	-10.695679	-7.109886	-1.362145
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	198	1	0	-7.346593	-9.977297	2.147839
	199	1	0	-12.240136	-9.623481	0.752511
	200	1	0	-12.539017	-9.308316	-0.956446
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	203	1	0	-13.311416	-11.564470	-0.288326
	204	1	0	-12.066092	-11.681109	-1.512885
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	207	6	0	-2.892788	-10.659736	0.411747
	208	6	0	-3.655872	-11.827306	0.261016
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	210	6	0	-5.019801	-11.834663	0.537821
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	215	1	0	-5.375166	-8.581643	1.477356
	216	6	0	-1.409063	-10.668442	0.190442
	217	6	0	-0.546758	-10.685812	1.307038
	218	6	0	-0.884020	-10.675877	-1.118818
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	245	1	0	2.975275	-8.580250	-0.956218
	246	1	0	3.168793	-12.746146	0.042603
	247	1	0	5.375166	-8.581643	-1.477356
	248	1	0	5.568873	-12.768164	-0.458935
	249	6	0	9.562207	-10.450579	-0.452988
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	253	6	0	11.397987	-12.248383	-0.470534
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	256	7	0	10.311867	-8.051905	0.172576
	257	1	0	9.690159	-10.161032	-1.500182
	258	1	0	10.161032	-9.690159	1.500182

	259	1	0	9.623481	-12.240136	0.752511
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	271	6	0	-10.659736	2.892788	0.411747
	272	6	0	-9.489664	3.549009	0.823927
	273	6	0	-11.827306	3.655872	0.261016
	274	6	0	-9.490944	4.911314	1.104269
	275	6	0	-11.834663	5.019801	0.537821
	276	1	0	-8.580250	2.975275	0.956218
	277	1	0	-12.746146	3.168793	-0.042603
	278	1	0	-8.581643	5.375166	1.477356
	279	1	0	-12.768164	5.568873	0.458935
	280	6	0	-10.668442	1.409063	0.190442
	281	6	0	-10.675877	0.884020	-1.118818
	282	6	0	-10.685812	0.546758	1.307038
	283	6	0	-10.685812	-0.546758	-1.307038
	284	6	0	-10.675877	-0.884020	1.118818
	285	6	0	-10.668442	-1.409063	-0.190442
	286	6	0	-10.678027	1.727231	-2.276687
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	289	6	0	-10.769732	-0.181268	-3.719432
	290	6	0	-10.743597	1.029140	2.652042
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	55	1	0	1.298648	5.315230	-2.186677
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	71	6	0	10.126208	0.824620	0.306020
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	105	1	0	-9.487831	2.574667 0.043170
	106	1	0	9.728438	1.717244 -0.187045

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