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Cyclopropanation reactions catalysed by dendrimers possessing one metalloporphyrin active site at the core: linear and sigmoidal kinetic behaviour for different dendrimer generations

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ABSTRACT

Experimental and computational studies on dendrimers possessing a Fe(porphyrin) catalytic core and polyether dendritic arms show that these macromolecules promote efficiently the (2+1) cycloaddition between a model alkene and diazomethane. The reaction is kinetically efficient and competitive with smaller catalysts. Lower generations of dendrimers exhibit a normal hyperbolic kinetic behaviour, whereas third- and fourth-generation dendrimers show a sigmoidal kinetic profile, compatible with cooperative effects most likely due to aggregation phenomena. This behaviour resembles that observed for Fe(porphyrin) containing biomolecules such as cytochromes and haemoglobin.

1. Introduction

Catalytic dendrimers[1] constitute an active research field, which has been intensively studied in the past two decades. These efforts have resulted in the development of novel catalysts possessing one metallic centre[2] and well-defined macromolecular organo-catalysts.[3] These macromolecular entities possess several interesting properties in homogeneous catalysis such as easier catalyst recovery by precipitation[4] or nano- and ultrafiltration.[5] Despite the fact that the separation of catalysts immobilized on solid supports will remain easier, there are other advantages of the dendritic approach. For example, higher overall activities of the homogenous systems, uniformity of catalyst structure and also the possibility of higher catalyst loading in the case of dendrimers with catalytic sites on the peripheries or branching points.

Installing a catalytic site onto a dendritic moiety either at the core or at the periphery can result in distinct catalytic properties with respect to polymeric or small molecule analogues. This variation has been termed as a 'dendrimer effect'.[6] In the case of core-functionalized dendrimers, the growth of the structure can enhance the catalytic performance by creation of tailored microenvironment in its centre. But also it can reduce the efficiency of the catalyst by rendering the central function hardly accessible for the substrate. Such activity decrease can be either successive,[7] or also abrupt, showing very similar behaviour for lower generations and swift downturn after a trespass of certain molecule size limit.[8] Quantitative measurements of dendrimer catalyst activity in dependence on the generation number are not very frequent; however, there are several examples of such studies,[9,10] showing different effects coming from dendron size to catalytic performance.

In previous work, we studied dendrimers with one active site[10,11] or one fluorophore[12] at the core. We observed negative, i.e., non-cooperative dendrimer effects with increasingly high

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generation numbers. Moreover, Morandi and Carreira[13] have recently published a very interesting study on the cyclopropanation of alkenes. We thought that this formal (2+1) cycloaddition[14] involving very reactive intermediates and relatively small substrates could be an interesting system to observe dendrimer effects in which the steric hindrance of the dendritic catalysts could be less relevant than in previously studied reactions.

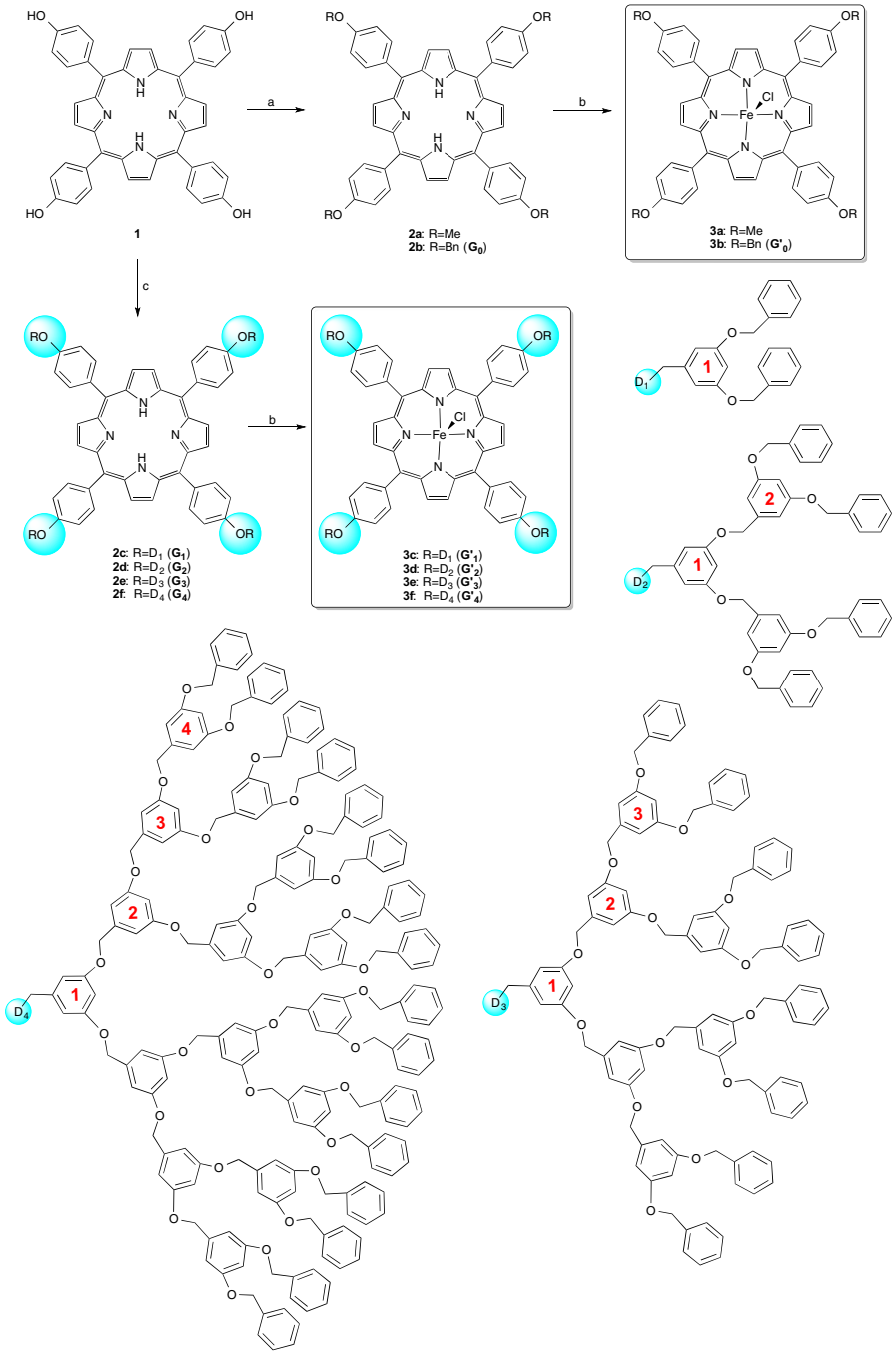
According to the Morandi–Carreira approach, the cyclopropanation of various styrene derivatives is performed in 6 M KOH in an open vial, with continuous addition of a water soluble diazomethane precursor, which provides this reactive intermediate under basic conditions, and under catalysis by Fe(III) tetraphenylporphyrin chloride (Fe(TPP)Cl) complex.[15] The approach successfully avoided hazardous isolation and handling of diazomethane.[16]

Within the context established by the precedents discussed above, in this paper we present our results on the dendrocatalytic version of the Morandi–Carreira reaction. In particular, we will focus our research on the catalytic behaviour of different generations of dendritic porphyrin-based[17] catalysts in order to assess the possibility of finding emergent properties for higher generations of these macromolecules.

2. Results and discussion

2.1. Synthesis of catalytic dendrimers

The general procedure followed for the synthesis of the catalysts is shown in Scheme 1 and was based on convergent strategy[18] for the synthesis of dendrimers. Thus, Fréchet-type disubstituted



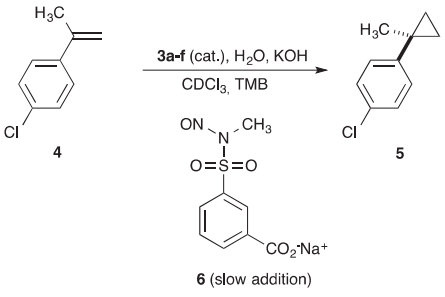
Scheme 1. Synthesis of dendrimeric catalysts **3a**–**f**. Reagents and conditions: a) K_2CO_3, DMF, MeI (for **2a**) or BnBr (for **2b**); b) $FeCl_2$, THF, O_2 (air); c) K_2CO_3, DMF, Br-D_n (n=1–4).

benzyloxy dendrons were prepared first up to the fourth generation. These dendritic wedges were obtained in the form of bromides (Br-D_n, n=1–4, see Scheme 1) following the original procedure.[19]

Subsequent conjugation of bromides Br-D_n with 5,10,15,20-tetrakis(4-hydroxyphenyl)porphyrin (TPP-$(OH)_4$, **1**) was carried out under conventional Williamson etherification conditions using K_2CO_3 as base and DMF as solvent, to yield dendrimeric porphyrins **2c**–**f** (generations **G1**–**G4**, see Scheme 1). Lower-weight analogous porphyrins tetrakis(4-methoxyphenyl)porphyrin **2a** and tetrakis(4-benzyloxyphenyl)porphyrin **2b** (0th generation dendrimer **G0**) were prepared for the shake of completeness and continuity using methyl iodide and benzyl bromide as Williamson electrophiles, respectively. Metallated porphyrins **3a**–**f** including dendrimer generations **G′0**–**G′4** were obtained by addition of ferrous chloride to porphyrins **2a**–**f** in refluxing solution of THF. Under these reaction conditions, Fe(II) intermediates were exposed to air and therefore the corresponding Fe(III)Cl-porphyrin derivatives[20] were obtained as stable compounds. Metallated porphyrins **3a**–**f** were characterized by HRMS (compounds **3a**–**c**) or by MALDI-TOF-MS (dendrimers **3d**–**f**) as well as by UV–visible spectroscopy. Non-metallated precursors **2a**–**f** were analysed by ^{1}H NMR and ^{13}C NMR spectroscopy (see the Experimental Section and the Supplementary data for further details).

2.2. Catalytic properties

Once we had prepared compounds **3a**–**f**, we studied their behaviour as catalysts in the cyclopropanation of substituted styrene **4** (1-chloro-4-(prop-1-en-2-yl)benzene) with diazomethane in deuterated chloroform. Following the Morandi–Carreira procedure,[13] diazomethane was generated *in situ* from 3-(*N*-methyl-*N*-nitrososulfamoyl)benzoate **6** (Scheme 2). The reaction mixtures were analysed by ^{1}H NMR using 1,2,3-trimethoxybenzene (TMB) as internal standard for the integration of the appropriate diagnostic signals corresponding to the internal standard, the reactant **4** and the (2+1) cycloadduct 1-(4-chlorophenyl)-1-methylcyclopropane **5** (Fig. 1).



Scheme 2. Cyclopropanation of styrene **4** (1-chloro-4-(prop-1-en-2-yl)benzene) with sodium 3-(*N*-methyl-*N*-nitrososulfamoyl)benzoate **6** catalysed by metalloporphyrins **3a**–**f**. TMB: 1,2,3-trimethoxybenzene.

According to the mechanism accepted for this kind of reactions, precursor **6** generates one equivalent of diazomethane in a solution of KOH in water (Scheme 3) with the concomitant formation of highly polar salt **7**, which remains in the aqueous phase. In situ formed diazomethane passes to the organic phase and reacts with the catalytic metalloporphyrin **3′** to yield the corresponding carbene–Fe complex. It has been proposed that reactive and unstable Fe(II) species are the actual active catalysts.[21] Indeed, it has been suggested[21a,c] that the diazomethane reactant can reduce the Fe(III)Cl complex **3** to the corresponding Fe(II) derivative **3′**. In addition, the Fe–carbene intermediate can exist in at least two

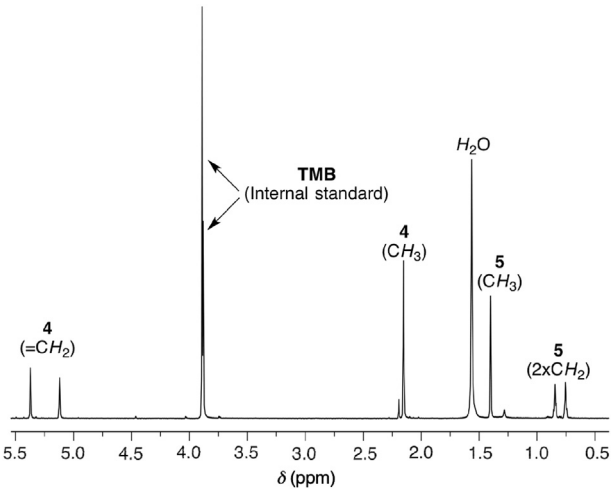
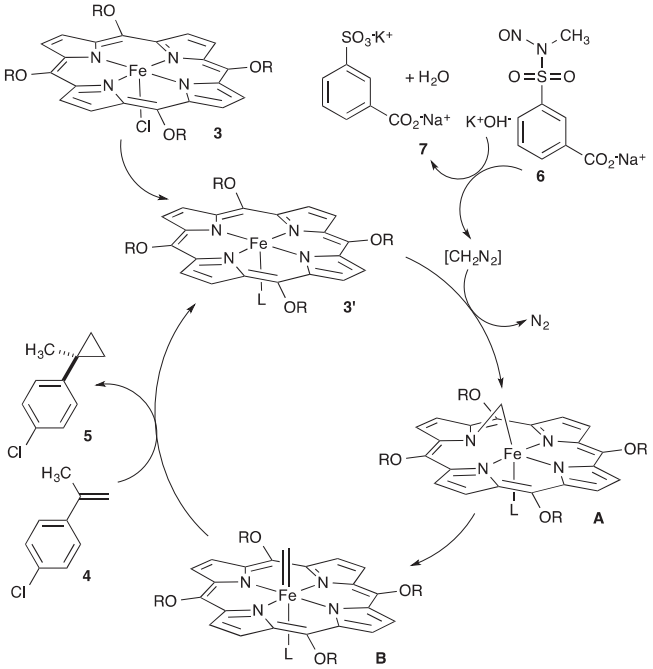


Fig. 1. Example of ^{1}H NMR spectrum recorded for the reaction between styrene **4** and in situ generated diazomethane to yield cyclopropane derivative **5** in the presence of catalyst **3b** (**G′0**, 2 mol %) at room temperature and after a reaction time of 40 min. TMB: 1,2,3-trimethoxybenzene.

different spin states as a bridged complex.[22] denoted as **A** in Scheme 3, which is in equilibrium with the corresponding axial isomer **B**. This latter intermediate interacts with the alkene to yield the (2+1) cycloadduct **5**, with the concomitant release of porphyrin **3′**, thus completing the catalytic cycle.



Scheme 3. Catalytic cycle for the cyclopropanation of alkene **4** to yield cyclopropane **5** in the presence of diazomethane precursor **6** and metalloporphyrins **3**.

The reaction was performed in a biphasic system (water/$CDCl_3$).[13] Using this approach, hydrophobic catalyst and substrate were dissolved in a small quantity of chloroform, which was vigorously stirred together with an aqueous solution of KOH. The reaction vessel was a flask that permitted a flow-off of excessive gas phase during the addition process through injected needle. Compound **6** was slowly added into the reaction system by means of an

automatic syringe, providing diazomethane under basic conditions. In situ generated diazomethane participated in the cyclopropanation reaction after its phase transfer into the droplets of chloroform. In the organic phase it was consumed by the metalloporphyrin catalyst **3** to form the corresponding metal–carbene intermediate, which reacted with the styrene substrate **4**. Due to the slow addition of **6**, diazomethane was present in the reaction system in substoichiometric quantity. On the contrary, the substrate in the organic phase was in local excess.

Since Morandi and Carreira[13] used a 2 mol % of Fe(TTP)Cl catalyst in the original work, we started our study on dendrimeric analogues by testing the **4**→**5** reaction with loadings of 1–10 mol % of Fe(TPP)Cl at an addition rate of 1 equiv of Fe(TTP)Cl per hour (Fig. 2). Experiments with 1, 2, and 4 mol % barely differed, while the experiment with 10 mol % showed lower performance (Fig. 2). This indicates that catalyst loads of 1–2 mol % were able to process the incoming diazomethane at very similar rate. Since precursor **6** and diazomethane were in a low ratio with respect to the substrate, higher catalyst loadings did not accelerate the reaction. However, consumption of substrate **4** took place at a rate lower than that associated with the instantaneous conversion of **6** into diazomethane and subsequent cyclopropanation of alkene **4** to form cyclopropane derivative **5**.

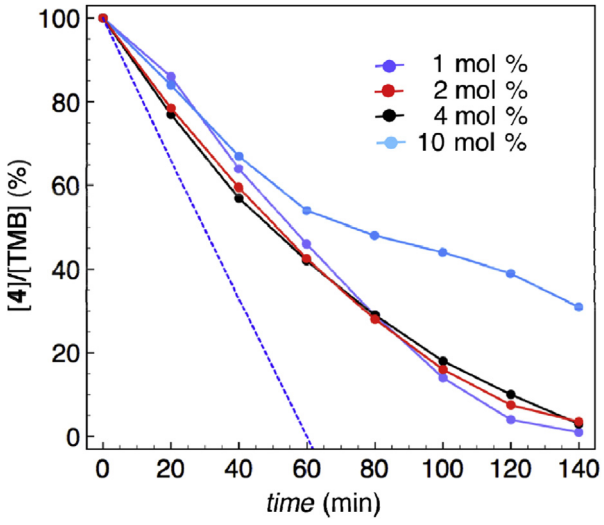


Fig. 2. Cyclopropanation of alkene **4** in $CDCl_3$ in the presence of Fe(TPP)Cl with different catalytic loads. Addition of diazomethane precursor **6** into KOH/H_2O solution was carried out at a rate of 1 equiv/h. The dashed line corresponds to the theoretical maximum reaction rate associated with conversion of **4** into cyclopropane derivative **5**, assuming instantaneous transformation of **4** into diazomethane and subsequent (2+1) cycloaddition on **4**.

The slow addition of diazomethane precursor **6** may raise questions about the promptness of decomposition of **6** or eventual accumulation of generated diazomethane in the reaction mixture. For this reason, we carried out an experiment to explore what the consequence of sudden cease of addition of **6** would be. Thus, we started the addition rate in the presence of substrate **4** and catalyst **3a** (2 mol %), with an addition rate of 1 equiv of **6** per hour. After 60 min of reaction time, we stopped this addition (Fig. 3). We observed that this interruption induces complete abortion of the reaction progress. This indicates that neither diazomethane nor its precursor **6** was accumulated in the reaction system, despite the less-than-optimal progress of the reaction (vide supra).

Considering the results of the latter experiment (Fig. 3), which show that only ca. 0.5 equiv of generated diazomethane were being

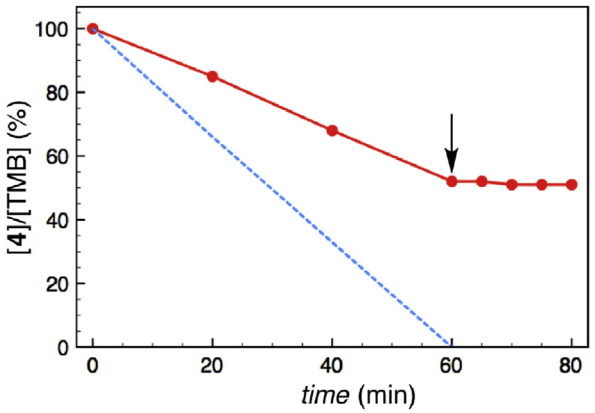


Fig. 3. Cyclopropanation of alkene **4** in $CDCl_3$ in the presence of catalyst **3a** (2% mol), with addition of diazomethane precursor **6** in KOH/H_2O at a rate of 1 equiv/h. The arrow indicates interruption of addition of **6**. The meaning of the dashed line is that indicated in Fig. 2 caption.

consumed in the formation of cyclopropane derivative, it can be assumed that at least some part of the remaining 0.5 equiv was constantly leaking away together with generated nitrogen. This escaping diazomethane was possibly passing directly to the gas phase instead of participating in the cyclopropanation in chloroform.

Experiments testing the performance of metalloporphyrin dendrimers **3b**–**f** (**G′0**–**G′4**) on the cyclopropanation reaction of alkene **4** using 2 mol % of catalyst were carried out under same conditions as described previously. Surprisingly, our results showed that the reaction progress was almost unvaried when Fe(TPP)Cl was replaced by simple metalloporphyrins **3a** and **3b** (**G′0**) and also by analogous dendrimers up to the second generation (**3c**, **3d**). However, the reaction rate decreased considerably with the transition to third- (**3e**) and fourth- (**3f**) generation dendrimeric catalysts (Fig. 4). The kinetic plots of catalysts **3e** and **3f** showed

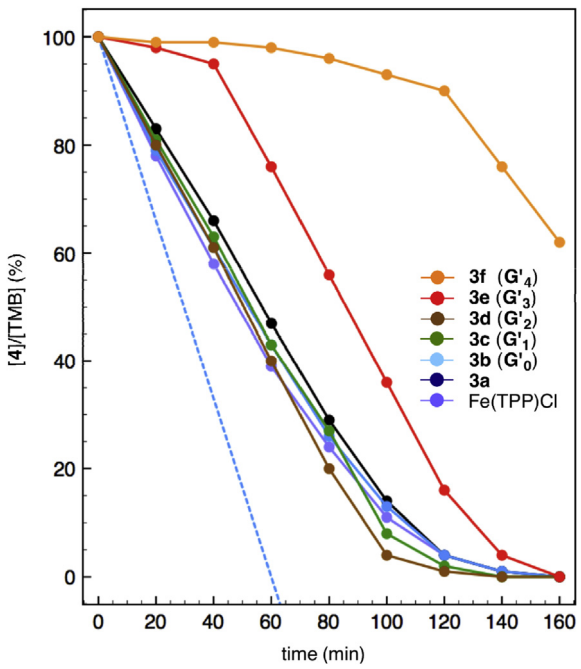


Fig. 4. Kinetic profiles corresponding to the conversion of alkene **4** into cyclopropane derivative **5** in the presence of catalysts Fe(TPP)Cl, **3a**, and **3b**–**f** (**G′0**–**G′4**). The reaction conditions are those reported in Fig. 2 caption.

sigmoidal character, with a relative latency at the beginning of the reaction, during, which the progress of the reaction was very slow. This period corresponded to 40 min for third-generation dendrimer **3e** and to 2 h for fourth-generation dendrimer **3f**. Surprisingly, after these induction times the reaction progresses accelerated to rates similar to those found for lower-generation catalysts (Fig. 4). In order to ensure that the catalytic activity of these dendrimers rely on the presence of the iron atom, additional blank test with non metallated dendrimers **2b**–**f** was carried out. As expected, no product formation was observed after 180 min under the described reaction conditions.

These results are compatible with a zero-order kinetic behaviour for substrate **4** under the slow injection conditions when small size catalysts are used. Thus, for first and second generation dendrimers **3c** and **3d** the kinetic profiles fit to zero-order kinetics for conversions up to 90% (the r^2 value was 0.998 in both cases, see Fig. 5) according to the following equation:

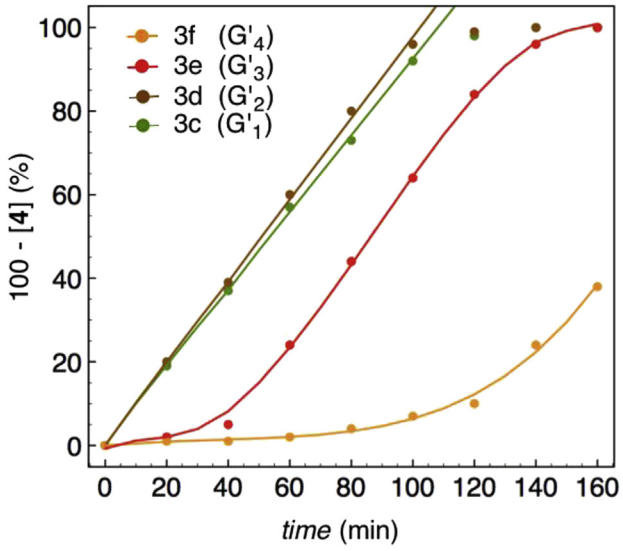


Fig. 5. Conversion profiles for catalytic dendrimers **3c**–**f**. Points correspond to experimental data and lines were obtained by means of Eq. 1 (**3c**,**d**) and (2) (**3e**,**f**).

$$100 - [4] = k_{obs}t \quad (1)$$

The values obtained for k_{obs} are 0.93 min^{-1} for **3c** (**G′1**) and 0.98 min^{-1} for **3d** (**G′2**), thus confirming the very similar catalytic ability of small dendrimers.

In the case of third and fourth generation dendrimers **3e** and **3f** the respective kinetic profiles were satisfactorily fitted[23] to a standard sigmoidal function of type $S(x)=1/(1+e^{-x})$ in the following form:

$$100 - [4] = \frac{100}{1 + exp[-\alpha(t-\tau)]} \quad (2)$$

The values obtained for the adjustable exponential parameter α decay on going from third to fourth generation catalysts. Thus, for third generation dendrimer **3e** it was found that α=0.051 min^{-1} and for its fourth generation congener **3f** the corresponding value is α=0.038 min^{-1}. The optimized induction time parameters τ were found to be quite different since for **3e** τ=87 min and in the case of **3f** τ=172 min. As a consequence, when catalyst **3e** is considered an almost linear zero order behaviour is reached for conversions between 20% (t=60 min) and 80% (t=120 min), with an apparent slope of 1.00 min^{-1}, a value very close to those found for **3c** and **3d**. In the case of fourth generation catalyst **3f**, the much larger induction time and the lower exponential factor result in a significantly lower catalytic ability.

In general, sigmoidal behaviour of kinetic plots can be due to two possible phenomena: autocatalysis[24] and cooperative effects.[25] In the former case, the sigmoidal kinetic profile stems from the acceleration[26] or inhibition[27] generated by the reaction product or by one reactant.[28] In our case, lower catalysts do not show this sigmoidal profile and the reaction product, namely cyclopropane derivative **5** is inert as far as the rate of the (2+1) process is concerned. Therefore, we reasoned that cooperative effects involving dendrimers **3d**,**f** are most likely due to aggregation processes. It is noteworthy that aggregation[29] and self-assembling[30] phenomena have been observed in dendrimers containing related cores such as phthalocyanines,[31] BINOL-Zn complexes,[32] and polyether dendrons.[12,33] In addition, it has been reported that the tendency to aggregation increases with the generation number of the dendrimer.[34]

We investigated the structural properties of metal-free dendrimers **2c**–**f** using molecular mechanics simulations[35] (see the Experimental Section) in order to get a better understanding of the experimentally observed catalytic effects. We optimized the starting geometries and sampled the different conformations by Molecular Dynamics (MD) simulations. Fig. 6 shows the shape of the most stable conformations at 298 K (within 4 kJ/mol) of dendrimers **2c** (**G1**) and **2d** (**G2**) in chloroform solution. The geometries thus obtained show that small reactants such as diazomethane and alkene **5** can reach the active site at the core of these dendrimers. This is due to one important feature of these dendrimers, namely the relatively long distance of ca. 16 Å between two collinear branching points at the periphery of the 5,10,15,20-tetraphenylporphyrin core.

In order to quantify the shape of dendrimers **2c**–**f** (**G1**–**G4**), we took the sphere and the cylinder as two extreme models. To do this, we first computed the radius of gyration[36] of each dendrimer of mass M and n-atoms of mass m_i as

$$R_g = \left[\frac{1}{M}\sum_{i=1}^{n} m_i\left(\vec{r_i} - \vec{g}\right)\left(\vec{r_i} - \vec{g}\right)\right]^{1/2} \quad (3)$$

where the position vector of the center of masses is given by

$$\vec{g} = \frac{1}{M}\sum_{i=1}^{n} m_i\vec{r_i} \quad (4)$$

The square of R_g can be expressed as the trace of the gyration tensor S in the form

$$R_g^2 = tr(S) = tr\begin{pmatrix} L_1^2 & 0 & 0 \\ 0 & L_2^2 & 0 \\ 0 & 0 & L_3^2 \end{pmatrix} \quad (5)$$

where the three components of the diagonalized tensor S are assigned as $L_1^2 > L_2^2 > L_3^2$. With these data, the asphericity[37] a_s of the dendrimer being considered is defined as

$$a_s = L_1^2 - \frac{1}{2}\left(L_2^2 + L_3^2\right) \quad (6)$$

For a perfect sphere, $L_1^2 = L_2^2 = L_3^2$ holds and hence a_s=0. Therefore, a_s quantifies the departure of the dendrimer from a perfect sphere. Similarly, acyclindricity[34] a_c can be defined as

$$a_c = L_2^2 - L_3^2 \quad (7)$$

Again, for a perfect cylinder a_c=0 since $L_2^2 = L_3^2$. Low values of a_c permit to identify a shape close to that expected for a cylindric

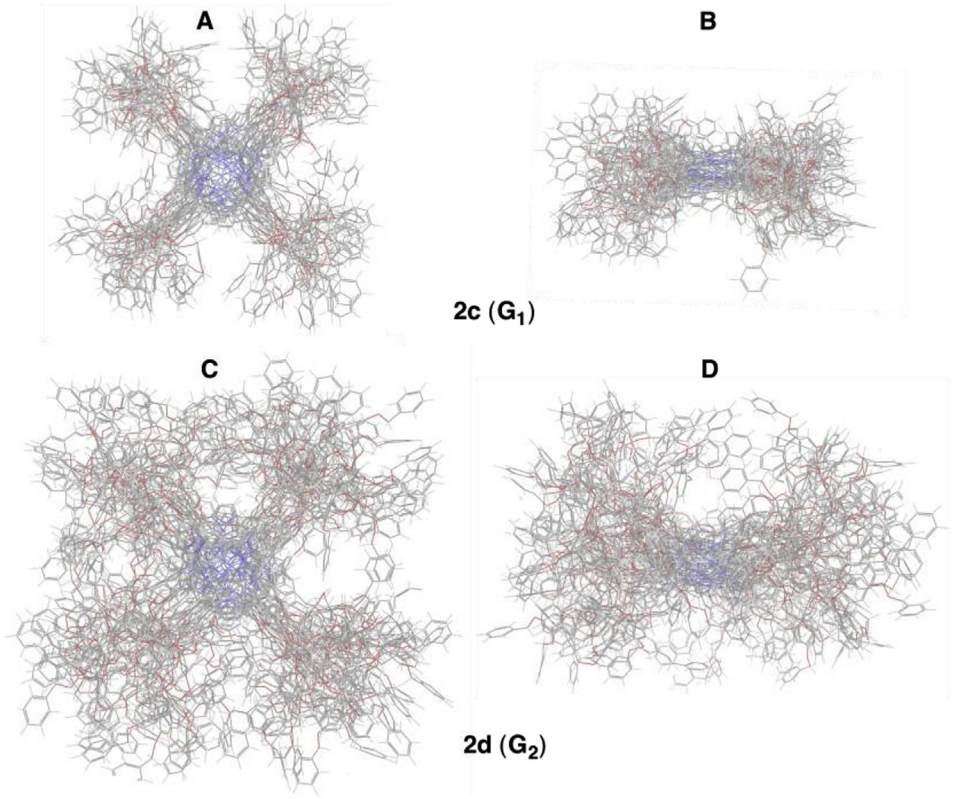


Fig. 6. Axial (A and C) and side (B and D) views of the most stable conformations (within 4 kJ/mol) of dendrimers **2c** (**G_1**, A and B) and **2d** (**G_2**, C and D) in chloroform solution. In all cases, porphyrin cores are highlighted in blue.

Table 1
Average values[a] of radii of gyration ($\langle R_g \rangle$, in Å), components of the diagonalized tensor S ($\langle L_i \rangle$, in Å), asphericities ($\langle a_s \rangle$, in Å^2) and acylindricities ($\langle a_c \rangle$, in Å^2) of dendrimers **2c**–**f** (**G_1**–**G_4**)

2c–**f**	$\langle R_g \rangle$	$\langle L_1 \rangle$	$\langle L_2 \rangle$	$\langle L_3 \rangle$	$\langle a_s \rangle$	$\langle a_c \rangle$
G_1	9.9±1.1	70.1±1.7	22.7±8.4	7.1±1.7	55.1±4.1	15.8±2.4
G_2	10.9±0.6	77.0±8.1	32.8±6.8	10.9±1.8	54.2±5.5	21.9±5.8
G_3	12.7±0.4	77.9±6.5	50.2±5.4	33.7±2.0	35.9±4.9	16.4±6.2
G_4	17.0±3.6	197.1±3.7	55.9±2.2	36.3±1.5	150.9±4.0	19.5±3.3

[a] Average values obtained from MD simulations after 1 ns of production time (see Fig. 7).

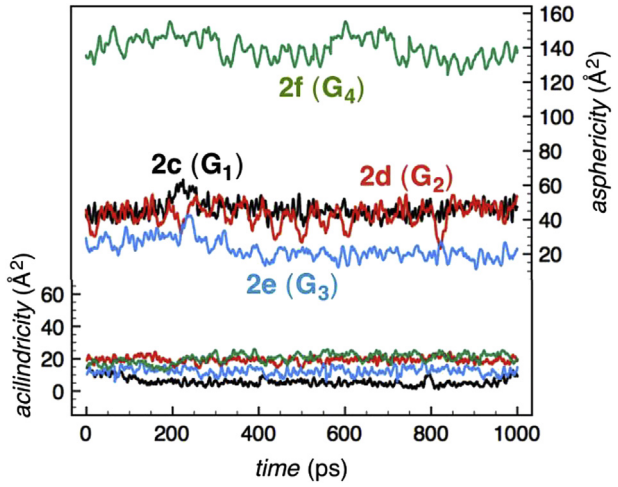


Fig. 7. Asphericities and acylindricities of dendrimers **2c**–**f** along the MD simulations.

molecular structure. The average values of R_g, a_s and a_c obtained along the MD simulations for **2c**–**f** are reported in Table 1. Asphericity and the evolution of the two latter magnitudes is gathered in Fig. 7.

Our results indicate that, in effect, the acylindricities for the different generations of dendrimers are quite similar, in agreement with the C_4 symmetry axis imposed by the porphyrin moiety. In addition, the asphericities of dendrimers **2c**–**e** (**G_1**–**G_3**) are quite similar and low. These results are compatible with the similar behaviour observed for **3c**–**e** with respect to **3b** (**G′$_0$**), **3a** and Fe(TPP)Cl. However, the similarities in acylindricity do not provide any clear explanation for the sigmoidal kinetic behaviour of **3e**,**f** (**G′$_3$**, **G′$_4$**). Since we hypothesized that cooperative effects leading to the

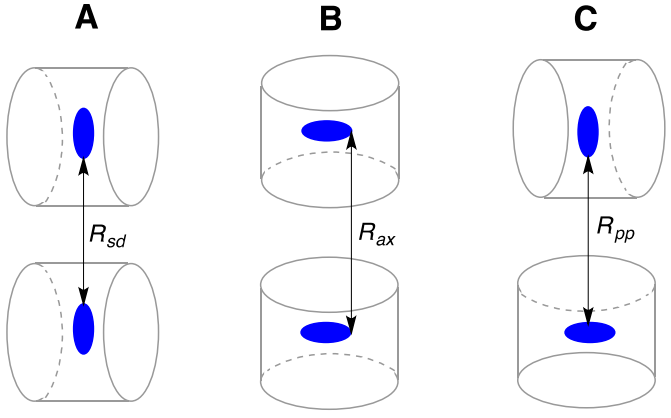


Fig. 8. Possible side (A), axial (B) and perpendicular (C) approaches for two units of cylinder-like dendrimers **2e**,**f** (**G_3**–**G_4**). R_{sd}, R_{ax} and R_{pp} denote the minimal distances between the two porphyrin rings.

formation of aggregates should cause this behaviour, we analysed the aggregation ability of dendrimers **2c** (**G$_1$**) and **2f** (**G$_4$**) by MD simulations in chloroform. At least three interaction models between cylinder-like dendrimers can be envisaged, as it is shown in Fig. 8. In the side and axial approaches, both dendrimers interact along parallel or collinear orientations of the two porphyrin systems, as shown in Fig. 8, whereas in the case of the perpendicular approach both porphyrin moieties interact along a T-shaped pattern. We tested the three interaction models for **G$_1$** and **G$_4$**. The results are gathered in Fig. 9.

Our MD simulations show that, after 50 ps of production time, the interacting units of **2c** (**G$_1$**) show a very low number of contacts between the two dendrimers even in the case of the axial pattern (Fig. 9). Actually, none of the three interaction patterns of **G$_1$** resulted to be dynamically stable, a result compatible with the presence of monomeric catalytic dendrimers **3c** and hence a normal kinetic behaviour in the cyclopropanation reaction. In contrast, fourth generation dendrimer **2f** showed a much slower motion after 50 ps of MD simulation, with dimeric structures of similar energies.

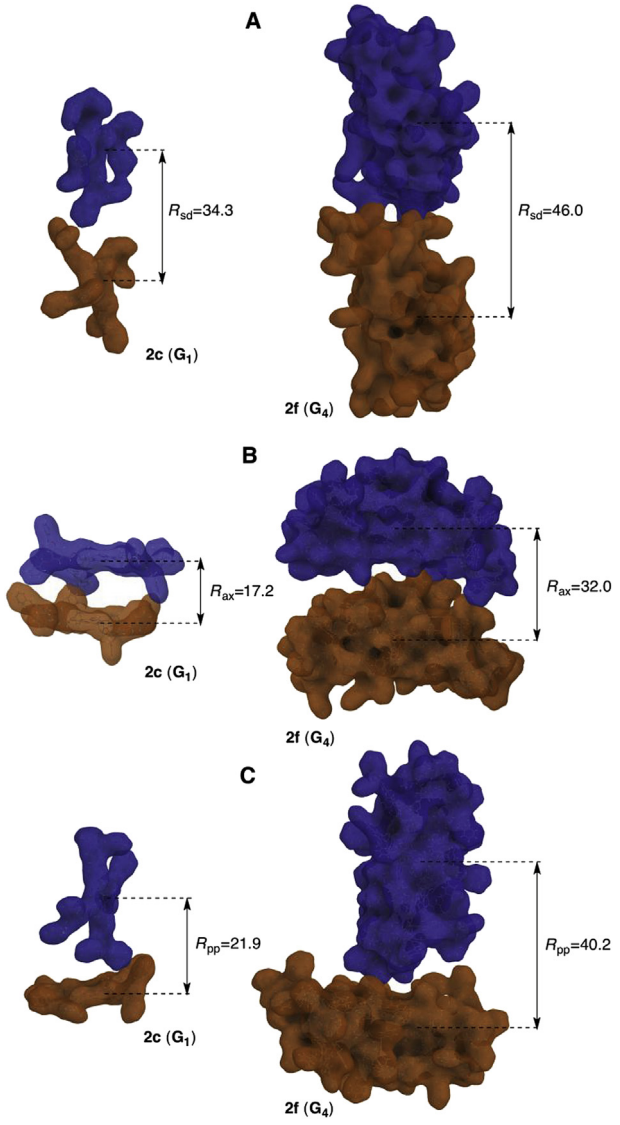


Fig. 9. Side (A), axial (B), and perpendicular (C) interaction models for dendrimers **2c** (**G$_1$**) and **2f** (**G$_4$**), after 50 ps of MD simulations in chloroform. Minimal porphyrin-porphyrin distances (see Fig. 7) are given in Å. Solvent accessible surfaces (SAS) are shown for the different dendritic units, with a probe radius of 1.4 Å.

Among them, axial and perpendicular interactions were persistent, the former offering more contact surface and shorter distances between the porphyrin moieties (Fig. 9). These results are compatible with persistent dimeric or, in general, oligomeric, structures of **2f** (**G$_4$**) and therefore for their Fe-containing catalysts **3f** (**G′$_4$**).

We confirmed the distinct aggregation patterns of **2c** and **2f** by performing further MD simulations under periodic boundary conditions (PBC) and with explicit treatment of the solvent. Thus, in the case of **2c** 3139 molecules of chloroform were included, whereas MD-PBC simulations with **2f** were carried out with a box of similar size including 1699 molecules of chloroform. The resulting ensembles were stabilized at 298 K and the respective calculations were run at constant temperature and volume for 2 ns.

Our results indicate that the axial dimer of **2c** is not stable: after 612 ps both monomeric structures move independently as in can be observed in Fig. 10A and B to reach an average R_{ax} distance of ca. 32 Å. This result confirms that the catalytic behaviour of **3c** (and those associated with low size analogues) can be understood in terms of monomeric intermediates along the catalytic cycle. In contrast, axial dimer of **2f** was stable along the production time, with an average R_{ax} value of ca. 27 Å that permits multiple van der Waals contacts between both dendrimeric units. Therefore, explicit treatment of the solvent compresses the dimeric structures and shows that these aggregates are not fleeting species. By extension, we concluded that fourth generation dendrimers could exist as dimers and higher order aggregates combining the three kinds of approaches shown in Figs. 8 and 9. On the basis of its similar sigmoidal behaviour, third generation dendrimers will exhibit a similar tendency to form aggregates.

To verify experimentally the different behaviour of metal free non-paramagnetic dendrimers **2c** and **2f**, we carried out different Diffusion-Ordered NMR Spectroscopy[38] (DOSY) experiments with these compounds at several concentrations in $CDCl_3$. We performed ^{1}H-DOSY experiments because of the high sensitivity of this technique, which permitted measurements at relatively low concentrations, especially in the case of fourth generation dendrimer **2f**. Fig. 11 shows the 2D spectra for both compounds, in which we have represented in the *x*-axis the part of the ^{1}H spectra corresponding to the benzylic signals associated with the Ar–CH_2–O moieties of both dendrimers. We observed that the relative diffusion rates for these signals were similar and easier to monitor at low concentrations (see the *y*-axes of Fig. 11). The respective diffusion coefficients are gathered in Table 2.

In the case of **2c** (**G$_1$**), we measured similar diffusion coefficients at relatively high concentrations of 11 mg/mL and 54 mg/mL. These values correspond to identical diffusion radii r_H estimated by means of the Stokes–Einstein[39] theory:

$$D = \frac{k_B T}{C\pi\eta r_H} \tag{8}$$

According to Eq. 8 the diffusion coefficient D varies inversely with the size of a hypothetical sphere of radius r_H. k_B is the Boltzmann's constant, η is the viscosity of the surrounding fluid (in our case chloroform, for which η=5.42×10^{-4} Pa/s at 298 K) and C is a constant that depends on the boundary conditions at the particle-solvent interface, and varies from C=6 to C=4 for spherical particles. From our NMR data we obtained for **2c** (**G$_1$**) the r_H value reported in Table 2 for C=4, which corresponds to approximate spheres associated with monomeric species moving under slip boundary conditions.[40] This result is in line with the radius of gyration of ca. 10 Å computed for monomeric **2c** (see Table 1). Therefore, on the basis of the ^{1}H-DOSY data, we concluded that, in agreement with our kinetic and MD data, first generation dendrimer **2b** (**G$_1$**) does not aggregate significantly, at least up to the highest concentration studied.

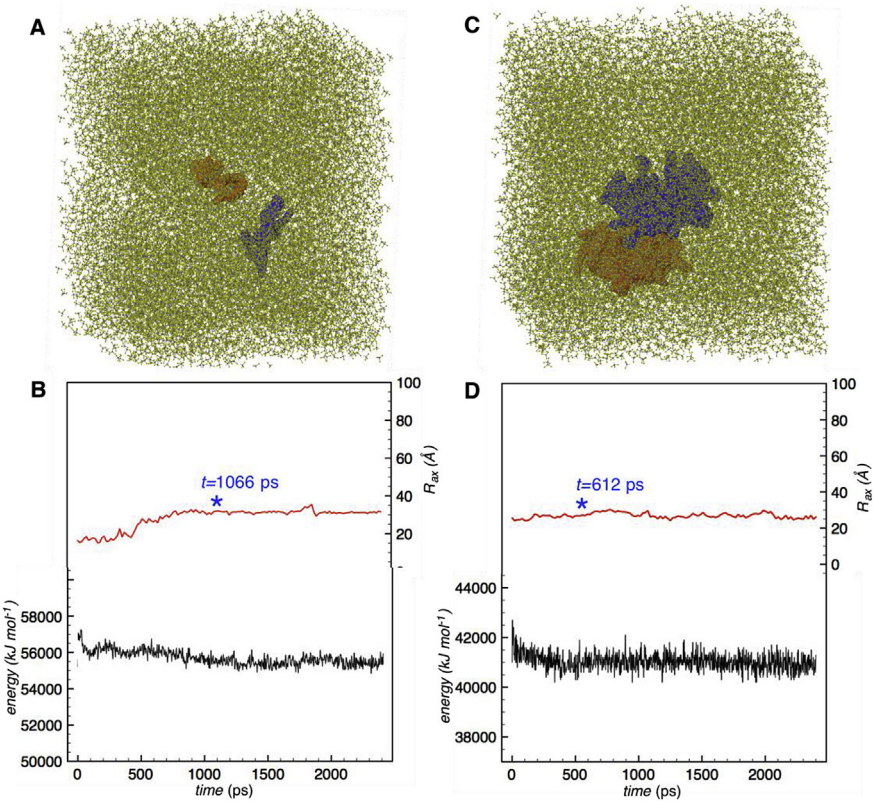


Fig. 10. MD-PBC simulations with axial dimeric structures of first and fourth generation dendrimers **2c** (A,B) and **2f** (C,D) in chloroform at 298 K. The solvent accessible surfaces (probe radius: 1.4 Å) for dimers of **2c** (A) and **2f** (C) are indicated. Snapshots gathered in (A) and (C) correspond to the production times indicated in (B) and (D), respectively. The energies and the R_{ax} values along production times for axial dimers corresponding to **2c** (B) and **2f** (D) are also shown.

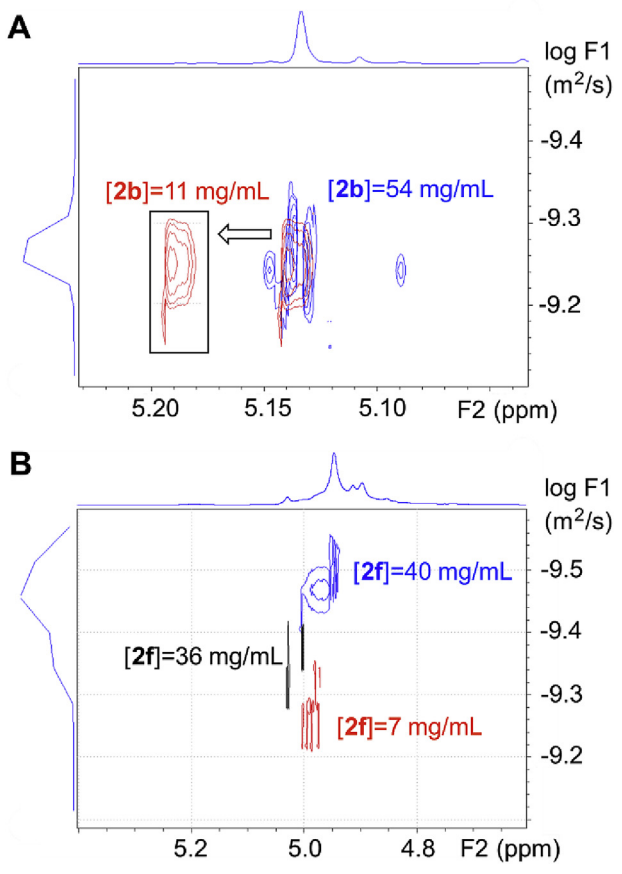


Fig. 11. 2D ^{1}H NMR data for dendrimers **2b** (A) and **2f** (B) in $CDCl_3$ at different concentrations. The inset in (A) corresponds to signals for **2b** at 11 mg/mL.

Table 2
Diffusion parameters of dendrimers **2c**,**f** (**G$_1$**,**G$_4$**)

Dendrimer	Conc. (mg/ml)	D (m^2/s)[a]	r_H (Å)[b]
2c (**G$_1$**)	11	5.44×10^{-10}	11.1
2c (**G$_1$**)	54	5.44×10^{-10}	11.1
2f (**G$_4$**)	7	4.76×10^{-10}	12.7
2f (**G$_4$**)	36	3.34×10^{-10}	18.1
2f (**G$_4$**)	40	2.51×10^{-10}	24.1

[a] Diffusion parameters D obtained by 2D ^{1}H-DOSY experiments.
[b] Diffusion radii estimated by means of the Stokes–Einstein equation with C=4.

The situation changed when the behaviour of dendrimer **2f** (**G$_4$**) was analysed at different concentrations (Table 2). In this case, we obtained different D values at different concentrations. Interestingly, the diffusion coefficients D obtained from the ^{1}H-DOSY experiments decreased, as the samples were more concentrated. At our lowest concentration of 7 mg/mL the r_H value was also the lowest one, slightly smaller than but comparable to-the average radius of gyration of ca. 17 Å. At our highest concentration of 40 mg/mL (we could not obtain accurate NMR spectra at higher concentrations because of solubility issues), the r_H value is of the same magnitude that (but slightly higher than) our computed radius for the dimer of **2f** (**G$_4$**), which was calculated to be of ca. 21 Å. On the basis of these results, we concluded that at the concentrations studied, higher generation dendrimer **2f** (**G$_4$**) forms dimers and, most likely, higher aggregates.

From our MD computational data and our DOSY NMR results, we interpret our kinetic experimental results in terms of the tendency of third and fourth generation dendrimers to form aggregates that result in a cooperative effect. First, higher generation dendrimeric aggregates capture the incoming diazomethane. The resulting intermediate carbene complexes can be buried inside the oligomeric structures and only after saturation of the aggregates the (2+1)

cycloaddition reaction starts to proceed efficiently. In addition, generation of more accessible Fe–carbene complexes on the surface of the aggregates and/or perturbation of the A–B equilibria (Scheme 3) and the corresponding preferred spin states cannot be ruled out. The final outcome is that these Fe–porphyrin aggregates show cooperative effects and sigmoidal kinetic plots similar to those observed in protein analogues such as cytochromes[41] and haemoglobin.[42]

3. Conclusions

In this work we report the preparation and assessment of the catalytic properties of different generations of dendrimers based on Fe(porphyrin) catalytic cores. These formally D_{4h}-symmetric dendrimers incorporate polyether Fréchet dendritic arms around the 5,10,15,20-tetrakis(4-hydroxyphenyl)porphyrin moiety. The reaction studied is the (2+1) cyclopropanation of a model alkene in the presence of diazomethane, safely and efficiently generated using the method reported by Morandi and Carreira. In contrast with the kinetic behaviour observed for other dendrimers with only one catalytic centre at the core, the reaction proceeds with rates comparable to those observed for the Fe(TPP)Cl catalyst. Thus, dendrimers from zeroth to second generation exhibit a normal linear pseudo zero order behaviour, with similar reaction rates. Structural parameters computed for these dendrimers are compatible with this result. In contrast, third and fourth generation dendrimers show sigmoidal kinetic plots, with increasing induction times on going from the third to the fourth generation. Beyond that point, the cyclopropanation reactions proceed and in the case of third generation catalyst the observed rate was comparable to those observed for lower generation catalysts. This distinct behaviour has been attributed to cooperative effects, generated via aggregation of dendritic units, a process that is only kinetically relevant for higher generations of dendrimers possessing large surfaces available for axial, side or perpendicular dendrimer-dendrimer contacts. This interpretation is compatible with molecular dynamics simulations. Finally, our results suggest that these macromolecules are efficient catalysts for the cyclopropanation of other alkenes under safe conditions, thus exploiting the advantages of dendrimers as catalysts.

4. Experimental section

4.1. General experimental methods

Reagents and solvents were purchased from commercial suppliers and used without further purification. Reagents used were of ACS reagent grade. Flash chromatography separations were carried out using silica gel 60 (0.040–0.063 mm) if not stated otherwise. NMR spectra were recorded at Varian Gemini 300 HC spectrometer or at Bruker Avance 500 spectrometer. HRMS (ESI+) spectra were recorded using LTQ Orbitrap Velos (Thermo Scientific) instrument. UV–vis spectra were recorded at Tecan Infinite 200 Pro spectrophotometer in range of 250–700 nm. Analytical TLC was performed on Merck TLC Silica gel 60 F_{254} plates using visualization by UV light at 254 nm and 365 nm. MS MALDI-TOF spectra were recorded on UltrafleXtreme MALDI-TOF/TOF mass spectrometer (Bruker Daltonics, Germany), using a 0.3 M solution of indoleacrylic acid in THF as matrix.

Water-soluble diazomethane precursor **6** was prepared following the procedure reported by Morandi and Carreira.[13] 3-(*N*-Methyl-*N*-nitrososulfam-oyl)benzoic acid (90 mg, 0.33 mmol, 90% purity) was suspended in water (2.7 ml) and $NaHCO_3$ (35 mg, 0.42 mmol) was added portionwise under stirring. The mixture was stirred for 1 h, filtered and the resulting solution of **6** was used immediately in kinetic experiment. Precursor 3-(*N*-methyl-*N*-nitrososulfamoyl)benzoic acid was purified by dissolution in a minimum quantity of dichloromethane, filtration and precipitation by pentane from the filtrate. The precipitate was dried under high vacuum. Its ^{1}H NMR analysis in methanol permitted to verify the ratio of nitrosation, comparing integrals of methyl group signals of this compound and its precursor 3-(*N*-methylsulfamoyl) benzoic acid. Using this method, 90% pure 3-(*N*-methyl-*N*-nitrososulfamoyl)benzoic acid was prepared, with remaining 10% of 3-(*N*-methylsulfamoyl)benzoic acid as impurity. Purified 3-(*N*-methyl-*N*-nitroso-sulfamoyl)benzoic acid was stored in a freezer under argon and was used in next few days in order to ensure unvaried purity of **6** in catalytic experiments. Otherwise, it was observed that 3-(*N*-methyl-*N*-nitrososulfamoyl)benzoic acid slowly decomposes by denitrosation back to 3-(*N*-methylsulfamoyl)benzoic acid if let at room temperature.

4.2. Procedures for the synthesis of metalloporphyrin catalysts

Polyaromatic Fréchet dendrons, of generation number one to four, Br-$D_{1\text{-}4}$, were prepared following the reported procedure. Their spectral properties were in accordance with those reported in the literature.[19] 5,10,15,20-Tetraphenylporphyrin iron(III) chloride (Fe(TPP)Cl) was prepared from commercial tetraphenylporphyrin as described previously.[15]

4.3. 5,10,15,20-Tetrakis(4-methoxyphenyl)porphyrin (2a)

Commercial 5,10,15,20-tetrakis(4-hydroxyphenyl)porphyrin **1** (100 mg, 0.147 mmol) was dissolved in DMF (3 ml). To this solution K_2CO_3 (200 mg, 1.45 mmol), 18-crown-6 (5 mg, 0.019 mmol) and iodomethane (1.14 g, 8.02 mmol, 0.5 ml) were added. Reaction mixture was protected from light and stirred for 20 h at 70 °C under argon. Then, the solvent was removed under reduced pressure. The resulting mixture was dissolved in CH_2Cl_2, filtered and deposed on a column of alumina (neutral, Brockman II). During the column separation 4% of THF in CH_2Cl_2 was used as mobile phase. After the precipitation by hexane from CH_2Cl_2, the title product was obtained as purple solid in 45% yield (64 mg, 0.066 mmol). Spectral properties of this compound were in accordance with those reported in the literature,[43] in which another procedure for the preparation of title compound is reported.

4.4. 5,10,15,20-Tetrakis(4-benzyloxyphenyl)porphyrin (2b)

5,10,15,20-tetrakis(4-hydroxyphenyl)porphyrin **1** (100 mg, 0.147 mmol) was dissolved in DMF (3 ml). To the solution K_2CO_3 (200 mg, 1.45 mmol), 18-crown-6 (5 mg, 0.019 mmol) and benzyl bromide (0.72 g, 4.21 mmol) were added. Reaction mixture was protected from light and stirred for 20 h at 70 °C under argon. Then, the solvent was removed under reduced pressure. The resulting mixture was dissolved in CH_2Cl_2, filtered, deposed on a column of alumina (neutral, Brockman II) and purified by column separation using 4% (v/v) of Et_2O in CH_2Cl_2 as mobile phase. After evaporation and precipitation with an appropriate hexane/CH_2Cl_2 mixture, the title product was obtained as a purple solid in 40% yield (58 mg, 0.056 mmol). Spectral properties of this compound were in accordance with those reported in the literature,[44] in which another procedure for the preparation of title compound is reported.

4.5. Porphyrin dendrimers 2c–e

These compounds were prepared from 5,10,15,20-tetrakis(4-hydroxyphenyl)porphyrin **1** and bromides Br-$D_{1\text{-}3}$ following the method reported by Matos, Fréchet et al. and their spectral properties were in accordance with the literature.[45]

4.6. Porphyrin dendrimer 2f

5,10,15,20-Tetrakis(4-hydroxyphenyl)porphyrin **1** (6.7 mg, 0.010 mmol) was dissolved in mixture of DMF (1 ml) and toluene (1 ml). To this solution K_2CO_3 (30 mg, 0.217 mmol), 18-crown-6 (5 mg, 0.019 mmol) and Br-D_4 (200 mg, 0.060 mmol) were added. The resulting reaction mixture was protected from light and stirred for 20 h at 70 °C under argon. Then, it was diluted by CH_2Cl_2 and extracted twice with brine. The organic phase was dried by $MgSO_4$, filtered and evaporated under reduced pressure. The residue was purified by flash chromatography on silica gel (toluene/CH_2Cl_2) and by precipitation with an appropriate mixture of hexanes/CH_2Cl_2 to afford the title product as purple glass in 36% yield (50 mg, 0.0036 mmol). ^{1}H NMR (500 MHz, $CDCl_3$): δ=−2.75 (s, 2H, N*H*), 4.82−4.93 (m, 224H, C*H*$_2$O), 4.97 (s, 16H, C*H*$_2$O), 5.13 (s, 8H, C*H*$_2$O), 6.41−6.71 (m, 172H, Ar−*H*), 6.83 (br s, 8H, Ar−*H*), 7.17−7.39 (m, 328H, phenyl H, phenylene H-3,5), 8.04 (d, 8H, phenylene H-2,6, *J*=7.6 Hz), 8.82 (s, 8H, porphyrin H). ^{13}C NMR (126 MHz, $CDCl_3$): δ=69.85, 69.95, 70.03 (CH_2O), 101.48, 106.29, 106.32, 106.38, 127.47, 127.49, 127.53, 127.91, 127.97, 128.47, 128.49, 128.55, 136.68, 139.15, 159.98, 160.05 (Ar, porphyrin, phenylene). UV−vis (THF) λ_{max}: 425 nm, 518 nm, 557 nm, 598 nm, 650 nm. MS (MALDI-TOF) *m/z* calculated 13,774.9 $[M+H]^+$, found 13,774.3.

4.7. General procedure for the synthesis of metalloporphyrins and dendrimers 3

The corresponding free-base porphyrin **2** and $FeCl_2$ were dissolved in dry THF and the reaction mixture thus obtained was refluxed under argon and under protection from light for 20 h. After cooling of the solution to room temperature, the mixture was exposed to open air under further stirring for 20 min. The solvent was evaporated and the obtained residue was purified by flash chromatography on silica gel, using CH_2Cl_2/MeOH as mobile phase, in order to remove unreacted $FeCl_2$. Observation of decay of Soret peak in measured UV−vis spectra permitted to monitor completion of iron insertion.[20a]

4.8. Metalloporphyrin 3a

The title compound was prepared as an orange-brown solid in 90% yield (92 mg, 0.815 mmol) from $FeCl_2$ (130 mg, 1.03 mmol), free-base porphyrin **2a** (100 mg, 0.096 mmol) and THF (30 ml). UV−vis (THF) λ_{max}: 414, 578, 620. HRMS (ESI+): *m/z* calculated 788.20805 $[M+H]^+$, found 788.20752. Preparation of this compound was reported previously[46] but spectral properties are unavailable in the literature.

4.9. Metalloporphyrin 3b (G_0)

The title compound was prepared as an orange-brown solid in 85% yield (160 mg, 0.0.085 mmol) from $FeCl_2$ (120 mg, 0.947 mmol), free-base porphyrin **2b** (40 mg, 0.054 mmol) and THF (12 ml). UV−vis (THF) λ_{max}: 412, 578, 620. HRMS (ESI+): *m/z* calculated 1092.33325 $[M+H]^+$, found 1092.33331. Preparation of this compound was reported previously[42] but spectral properties are unavailable in the literature.

4.10. Metalloporphyrin 3c (G_1)

The title compound was prepared as an orange-brown solid in 76% yield (128 mg, 0.0647 mmol) from $FeCl_2$ (110 mg, 0.868 mmol), free-base porphyrin dendrimer **2c** (160 mg, 0.0.085 mmol) and THF (25 ml). UV−vis (THF) λ_{max}: 412, 576, 616. HRMS (ESI+): *m/z* calculated 1941.67152 $[M+H]^+$, found 1941.67040.

4.11. Metalloporphyrin 3d (G_2)

The title compound was prepared as an orange-brown solid in 90% yield (125 mg, 0.0340 mmol) from $FeCl_2$ (100 mg, 0.785 mmol), free-base porphyrin dendrimer **2d** (135 mg, 0.0375. mmol) and THF (21 ml). UV−vis (THF) λ_{max}: 423, 582, 616. MS (MALDI-TOF): *m/z* calculated 3639.9 $[M]^+$, found 3640.2, loss of C_7H_6 (calcd *m/z* 3549.9, found 3549.8).

4.12. Metalloporphyrin 3e (G_3)

The title compound was prepared as an orange-brown solid in 96% yield (35 mg, 0.0025 mmol) from $FeCl_2$ (100 mg, 0.785 mmol), free-base porphyrin dendrimer **2e** (115 mg, 0.0165 mmol) and THF (25 ml). UV−vis (THF) λ_{max}: 422, 506 (very weak), 576 (very weak). MS (MALDI-TOF): *m/z* calculated 7035.9 $[M]^+$, found 7035.4; loss of C_7H_6 (calcd *m/z* 6945.8, found 6945.9).

4.13. Metalloporphyrin 3f (G_4)

The title compound was prepared as an orange-brown solid in 75% yield (112 mg, 0.0158 mmol) from $FeCl_2$ (25 mg, 0.197 mmol), free-base porphyrin dendrimer **2e** (45 mg, 0.0033 mmol) and THF (5 ml). UV−vis (THF) λ_{max}: 424, 508 (very weak), 582 (very weak). MS (MALDI-TOF): *m/z* calculated 13,827.7 $[M]^+$, found 13,853.1.

4.14. General procedure for the kinetic experiments with catalysts 3a–d

A solution of 1-chloro-4-(prop-1-en-2-yl)benzene **4** (16.7 mg, 0.110 mmol, 0.016 ml), 1,2,3-trimethoxybenzene (internal standard, 10 mg, 0.059 mmol) and the corresponding metalloporphyrin catalyst **3a**–**d** (2 mol%, 0.0022 mmol) in $CDCl_3$ (0.4 ml) was added to an aqueous solution of KOH (6 M, 1 ml) in a 5 ml flask sealed with a septum. The resulting biphasic mixture was vigorously stirred for 5 min. Then, keeping the magnetic stirring, slow addition of freshly prepared aqueous solution of diazomethane precursor **6** (0.122 M, 2.7 ml) was started using an automatic syringe pump, keeping the addition rate at 0.9 ml/h, which corresponds to 1 equiv of **6** per hour. At the start of the addition, an open 1 ml plastic syringe without plunger, previously filled with a KOH solution (6 M, 0.3 ml), was introduced into the flask via needle to lead off excess of gas phase during the addition process. Aliquots of 0.020 ml were withdrawn from the organic phase by means of a microsyringe after a short cease of stirring. The aliquots were withdrawn every 20 min after the start of the addition of **6** solution and also shortly before starting the experiment. The aliquots were diluted by $CDCl_3$ to stop the reaction and analysed by ^{1}H NMR. The reaction progress was monitored by calculation of substrate concentration decrease from the NMR data of the crude reaction mixture. Integrals of the ^{1}H NMR signal of the substrate methyl group (δ, ppm: 2.12) in each sample were compared with the integral of internal standard methyl groups (δ, ppm: 3.87, 3.86), using the aliquot taken before starting the addition of **6** as reference.

Blank experiments were performed under identical conditions but in the absence of catalysts **3**. No reaction progress was observed during the time of 3 h.

Experiment with interruption of the addition of diazomethane precursor **6** was carried out by following the general procedure using metalloporphyrin **3a** as catalyst, but the addition of **6** solution was stopped after 60 min. Since that moment, aliquots were withdrawn every 5 min during the next 20 min. No significant reaction progress was observed after interruption of the addition of **6**.

4.15. Procedure for the kinetic experiments using 3e or 3f as catalysts

Under the conditions reported for the previous general procedure, metallodendrimers **3e** and **3f** formed emulsions when stirred in the biphasic system, which could result in a slower progress of the reaction. To avoid the formation of emulsions, the flask size was changed from 12×45 mm to 15×55 mm and the size of the magnetic stirrer bar from 5×12 mm to 8×12 mm. The amount of $CDCl_3$ used was increased to 0.6 ml.

4.16. 1,2,3-Trimethoxybenzene (internal standard)

This compound is commercially available and was used without further purification. ^{1}H NMR (500 MHz, $CDCl_3$): δ=3.86 (s, 3H, OCH_3), 3.87 (s, 6H, OCH_3), 6.59 (d, 2H, ArH), 7.00 (t, 1H, ArH).

4.17. 1-Chloro-4-(prop-1-en-2-yl)benzene (4)

This compound is commercially available and was used without further purification. ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.12 (s, 3H, $-CH_3$), 5.09 (s, 1H, $=CH_2$), 5.34 (s, 1H, $=CH_2$), 7.28 (d, 2H, ArH, J=8.51 Hz), 7.38 (d, 2H, ArH, J=8.80 Hz).

4.18. 1-Chloro-4-(1-methylcyclopropyl)benzene (5)

This (2+1) cycloadduct was obtained as colourless oil by column chromatography from the different reaction mixtures following the general procedure for kinetic experiments. Spectral properties are in accordance with those reported in the literature.[13] ^{1}H NMR (500 MHz, $CDCl_3$): δ=0.70–0.75 (m, 2H, CH_2), 0.80–0.84 (m, 2h, CH_2), 1.38 (s, 3H, CH_3), 7.14–7.24 (m, 4H, Ar*H*).

4.19. ^{1}H-DOSY experiments

The different experiments were carried out on a Bruker 500 AVANCE equipped with a *z*-gradient BBO probe. Each DOSY experiment was recorded using the *lebbpgp2s* sequence. The number of scans was 16. The strength of the gradient was changed from 2 % to 95% using a 50 G/cm gradient unit. The value of big delta Δ was 200 ms and little delta δ was 800 ms. A delay of 5 ms was used to avoid the formation of eddy currents.

4.20. Computational methods

All the computational studies reported in this paper were based upon molecular mechanics[47] (MM) and molecular dynamics (MD).[48] In both, the MM3 method developed by Allinger et al. as implement in the MacroModel[49] package was used. All MD simulations were performed with SHAKE[50] to constrain the C–H bonds. The temperature was set up to 298 K. The system was equilibrated for 1 ns with time steps of 1 fs. This equilibration time is 10 times longer than the expected value for the relaxation time of dendrimers[51] of this size. The production run was started from this point and lasted another nanosecond with time steps of 1 fs. In all cases, we observed that during the production period, the energy and temperature of the whole system were equilibrated. During the production run, the coordinates were saved each picosecond, which implies a total of 1000 structures. These structures were used to calculate the averages of the properties specified below. To calculate these properties, programs based on the DYNAMO library[52] were written. In the case of MD simulations under periodic boundary conditions (MD-PBC) in chloroform, a specific force field potential optimized for liquid simulations (OPLS_2005)[53] was used as implemented on Desmond package.[54] These simulations were performed using periodic boundary conditions within the canonical NVT ensemble at 298.15 K and a cubic box of 90 Å of side length. The system was equilibrated for 2 ns with time steps of 1 ps.

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Supplementary data

Supplementary data associated with this article can be found in the online version, at http://dx.doi.org/10.1016/j.tet.2016.01.013.

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Cyclopropanation reactions catalysed by dendrimers possessing one metalloporphyrin active site at the core: linear and sigmoidal kinetic behaviour for different dendrimer generations

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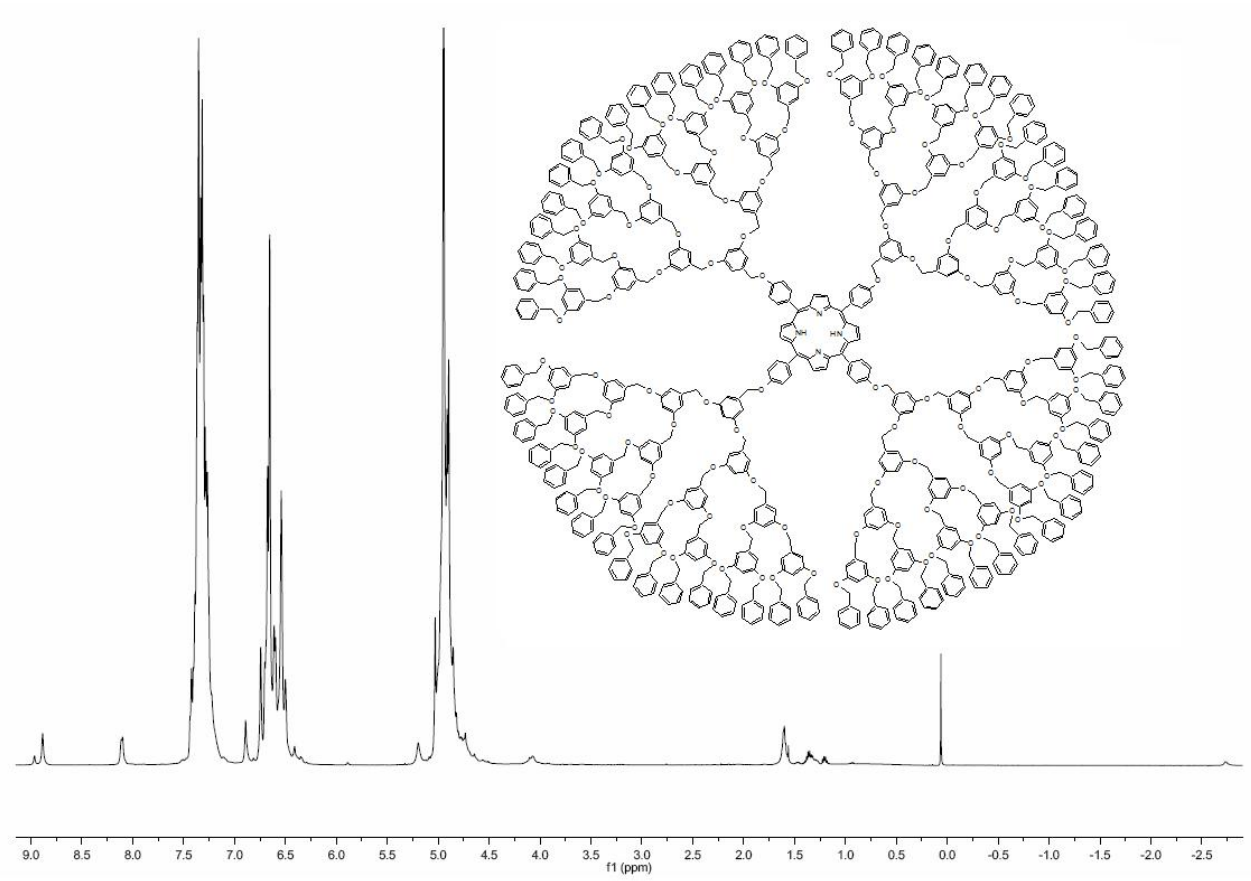
Supporting Information

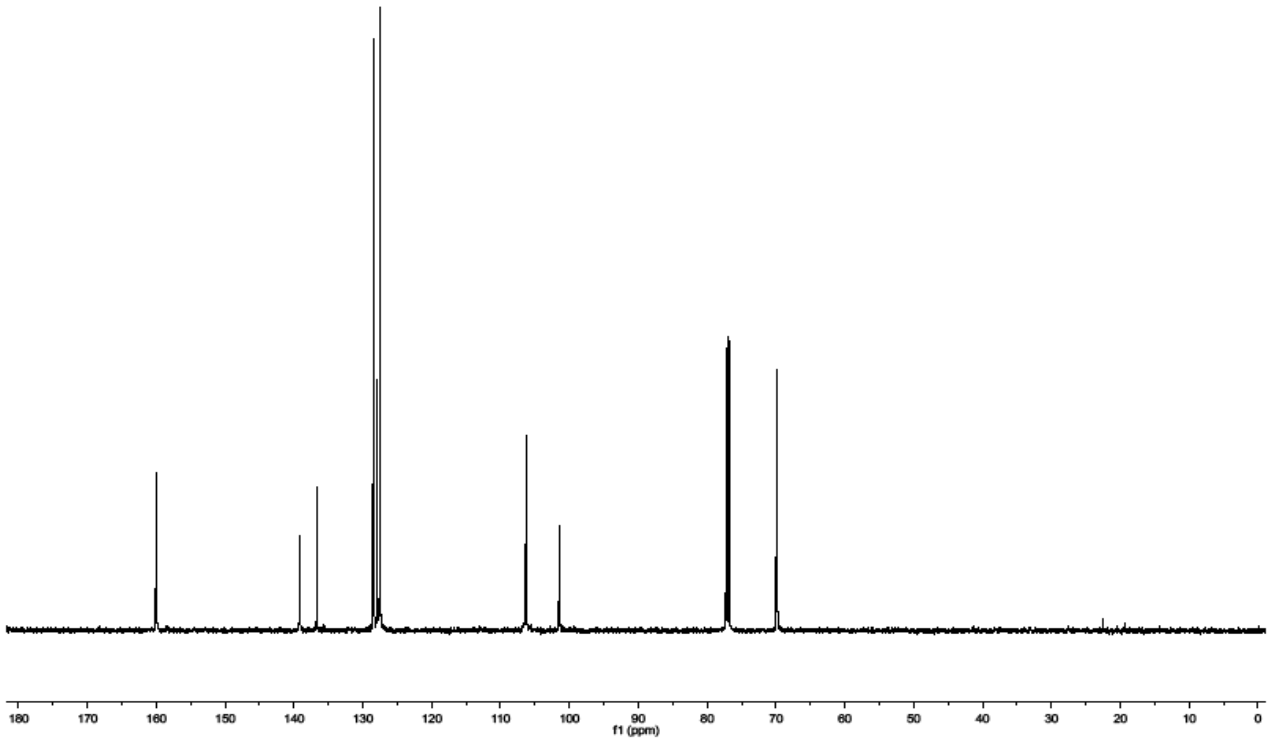
List of Contents:

1. ^{1}H NMR AND ^{13}C NMR SPECTRA OF NEW COMPOUNDS

^{1}H NMR ($CDCl_3$) **2f**



^{13}C NMR ($CDCl_3$)) **2f**



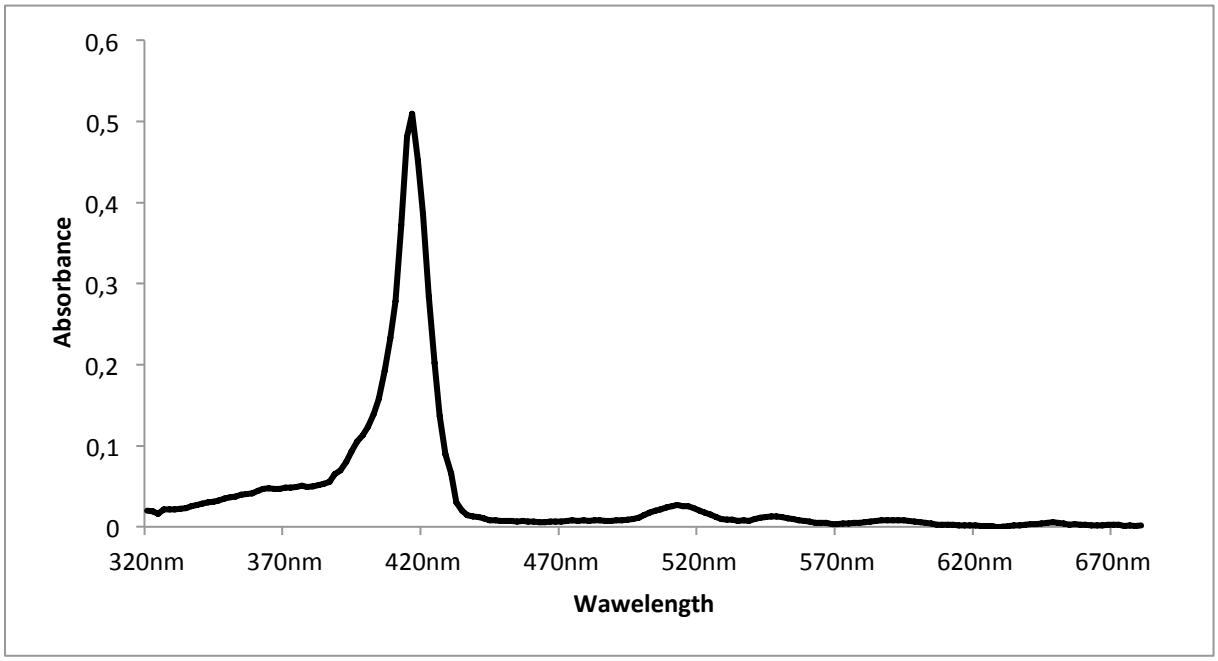
As expected from earlier results, the NMR spectra of new metallodendrimers prepared (**3c–f**) were broadened by the effect of paramagnetic high-spin Fe(III) present in the porphyrin core. (ref.: X. Zheng, I. R. Oviedo, L. J. Twyman: *Macromolecules* **2008**, *41*, 7776)

2. UV-vis spectra of metalloporphyrins and their free-base precursors

Spectra of 1 . 10^{-6} M solutions of porphyrins in THF were measured in standard 1 cm UV cuvette, with slit width of the spectrometer of 2 nm. The positions of maxima of Soret peaks of free-base porphyrins were recorded with a slit width of 1 nm.

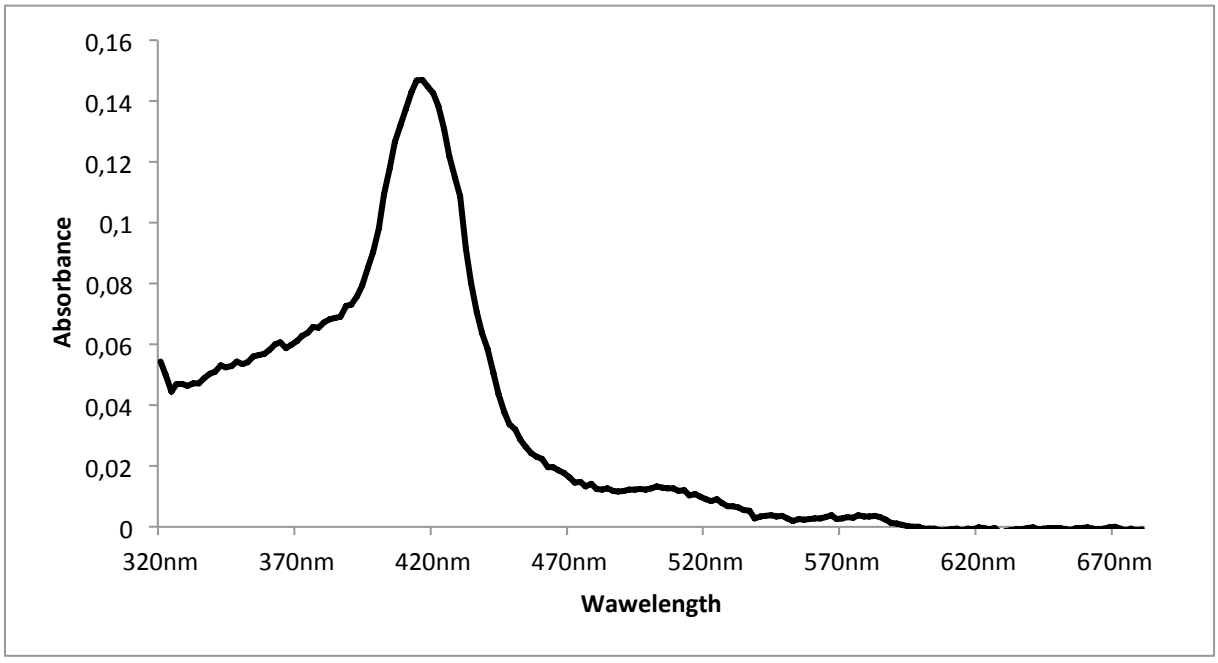
5,10,15,20-Tetraphenylporphyrin (TPP)

λ_{max} (log ε): 416 nm (5.71), 512 nm (4.43), 548 nm (4.11)

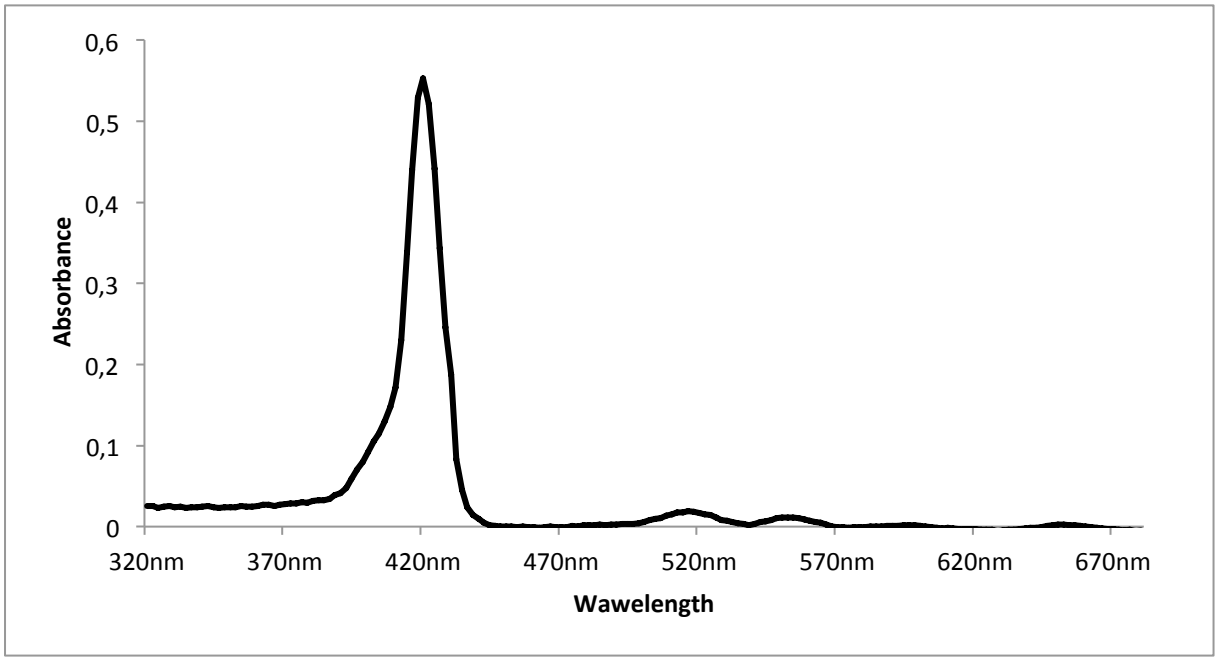


Fe(TPP)Cl

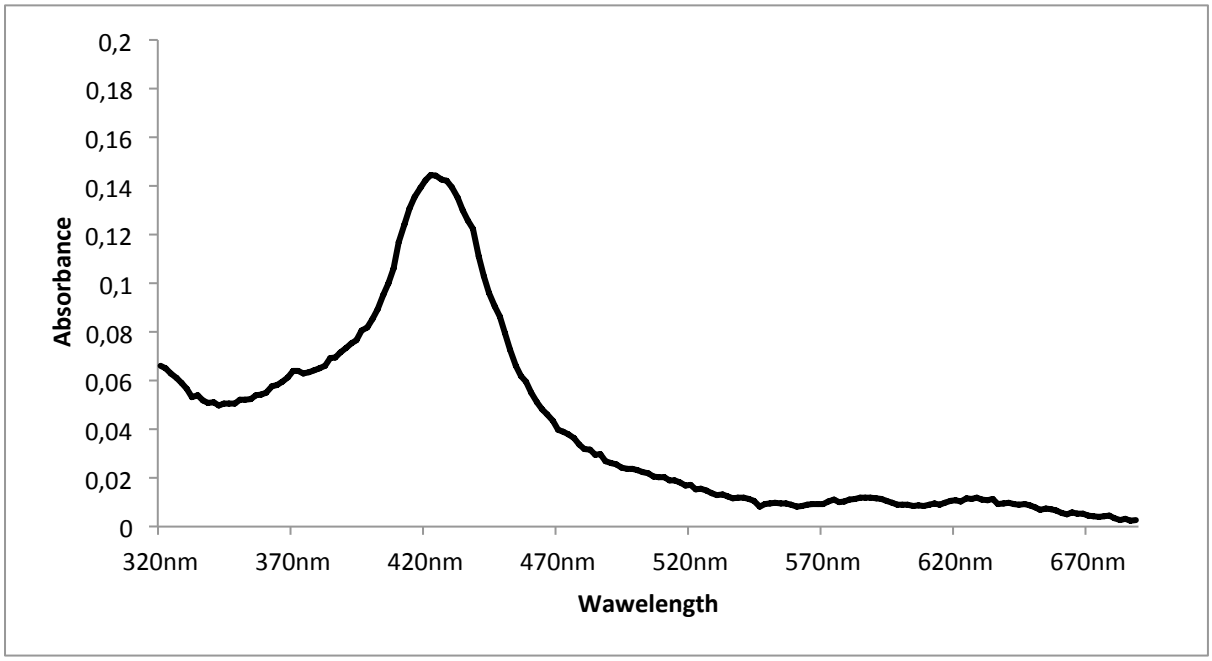
λ_{max} (log ε): 416 nm (5.17), 502 nm (4.12), 576 nm (3.58)



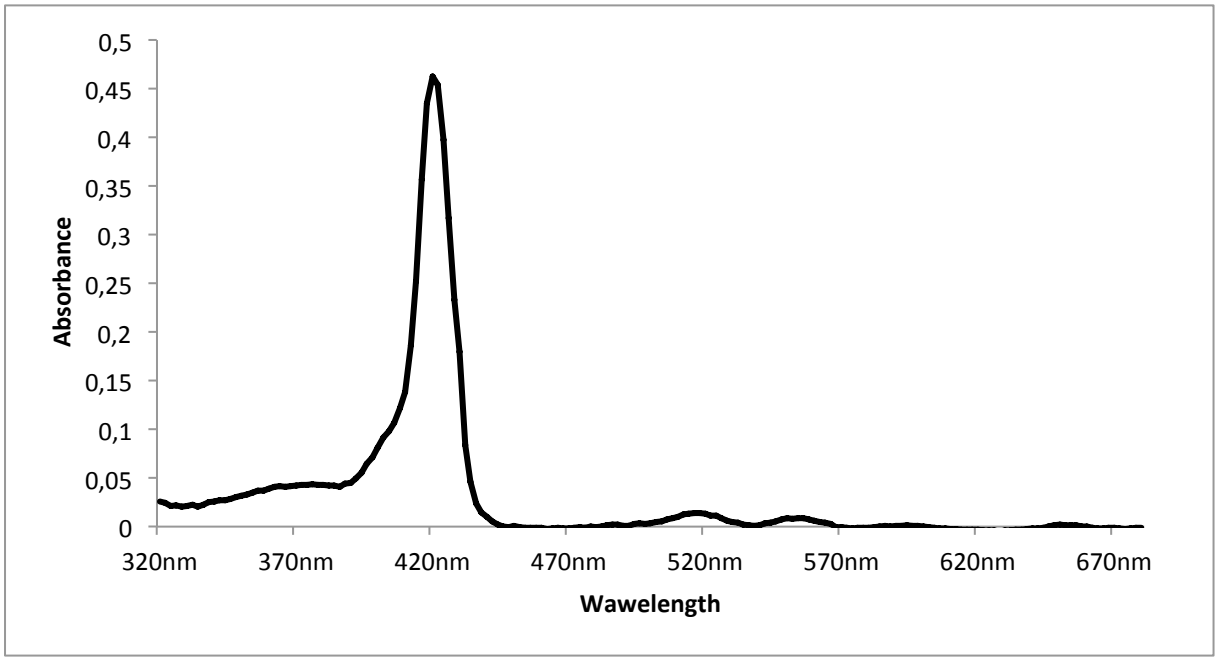
5,10,15,20-Tetrakis(4-methoxyphenyl)porphyrin – **2a**
λ_{max} (log ε): 420 nm (5.74), 516 nm (4.28), 554 nm (4.05)



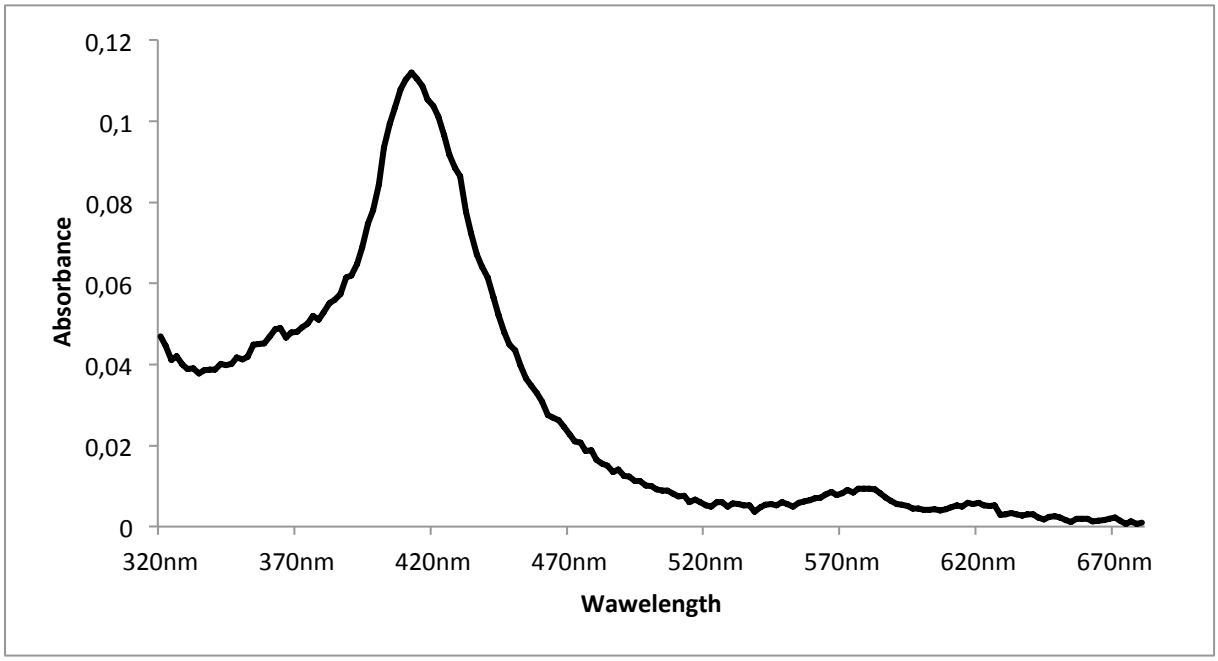
Metalloporphyrin **3a**
λ_{max} (log ε): 414 nm (5.16), 578 nm (4.08), 620 nm (4.08)



5,10,15,20-Tetrakis(4-benzyloxyphenyl)porphyrin – **2b**
λ_{max} (log ε): 421 nm (5.67), 516 nm (4.15), 554 nm (3.93)

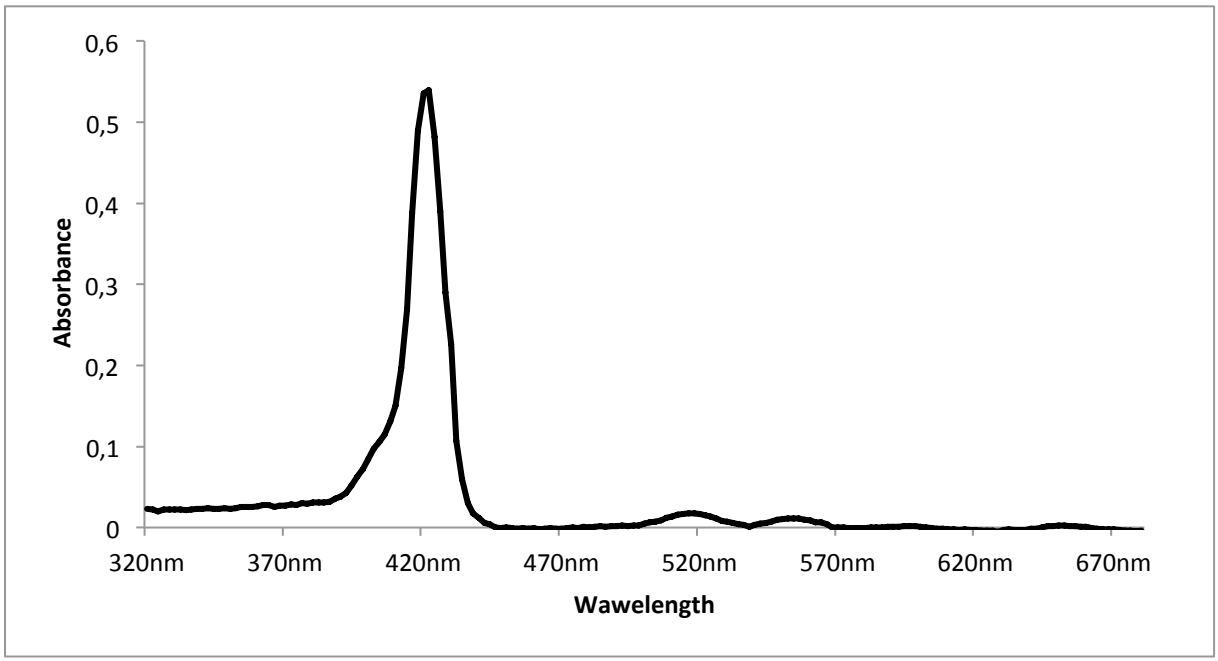


Metalloporphyrin **3b**
λ_{max} (log ε): 412 nm (5.05), 580 nm (3.97), 620 nm (3.77)



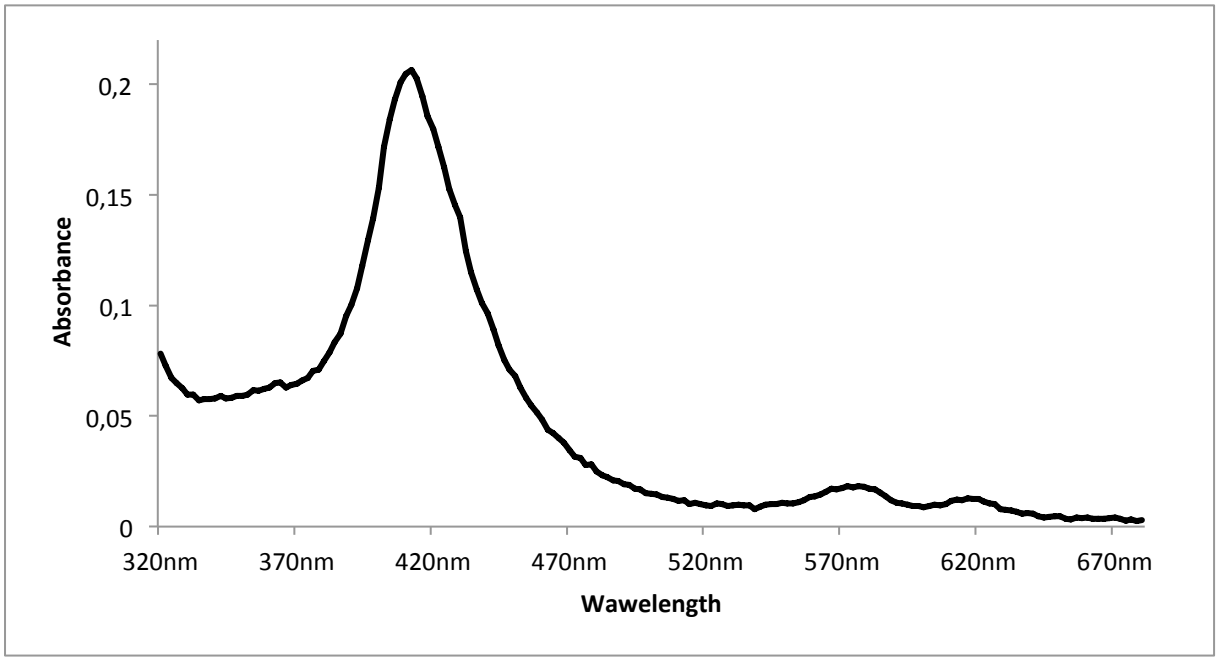
Dendrimer **2c**

λ_{max} (log ε): 421 nm (5.73), 516 nm (4.25), 556 nm (4.06)



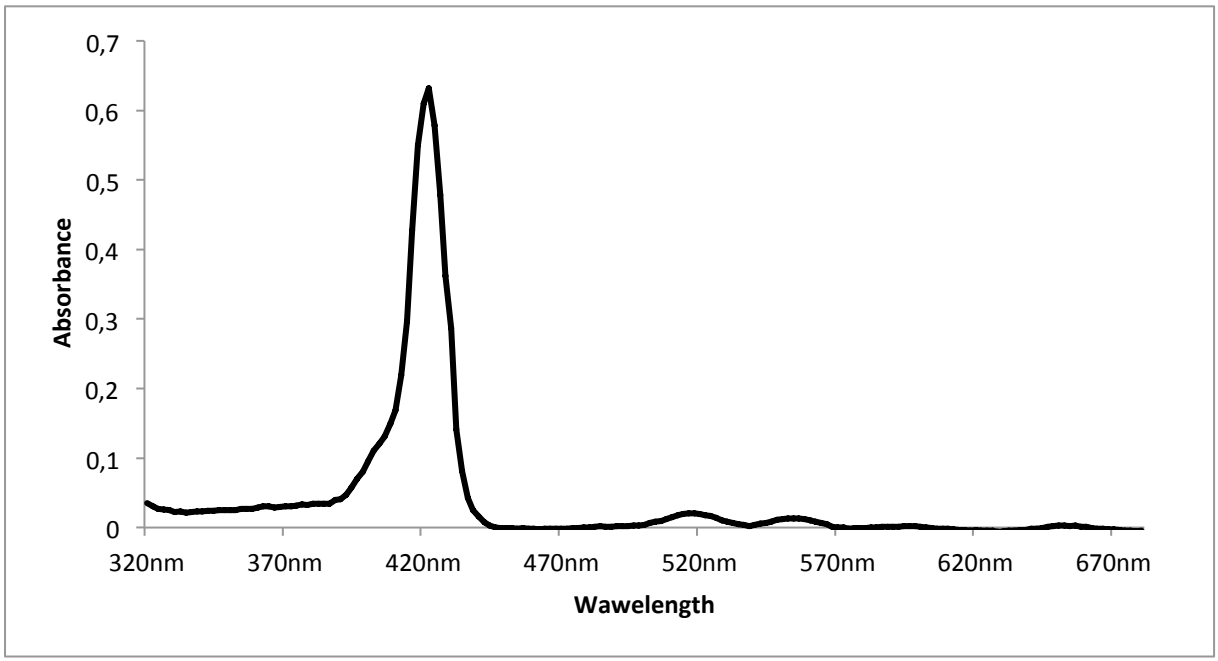
Dendrimer **3c**

λ_{max} (log ε): 412 nm (5.31), 576 nm (4.26), 616 nm (4.10)



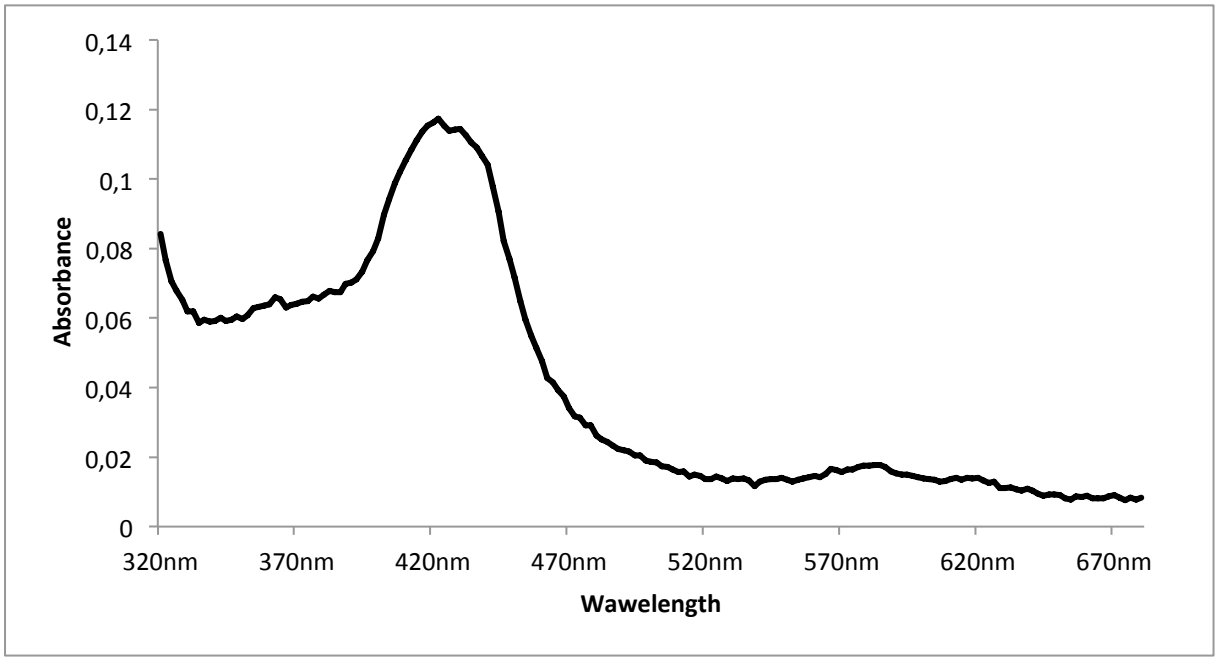
Dendrimer **2d**

λ_{max} (log ε): 421 nm (5.80), 516 nm (4.32), 556 nm (4.13)



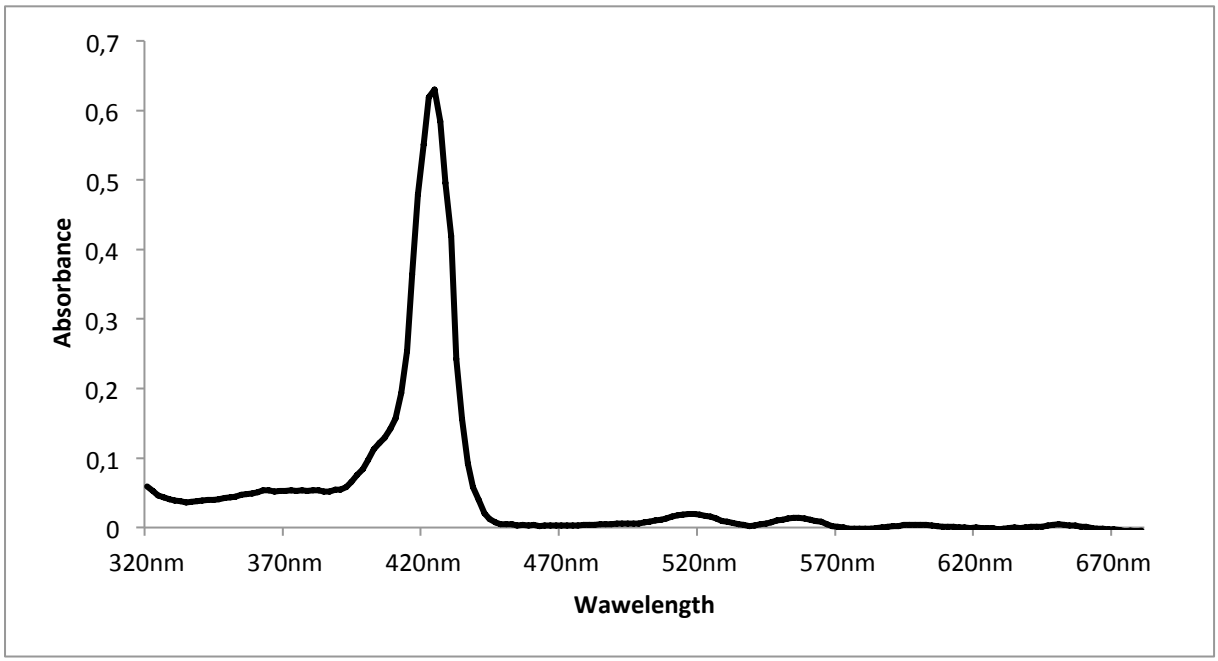
Dendrimer **3d**

λ_{max} (log ε): 422 nm (5.07), 582 nm (4.25), 616 nm (4.15)



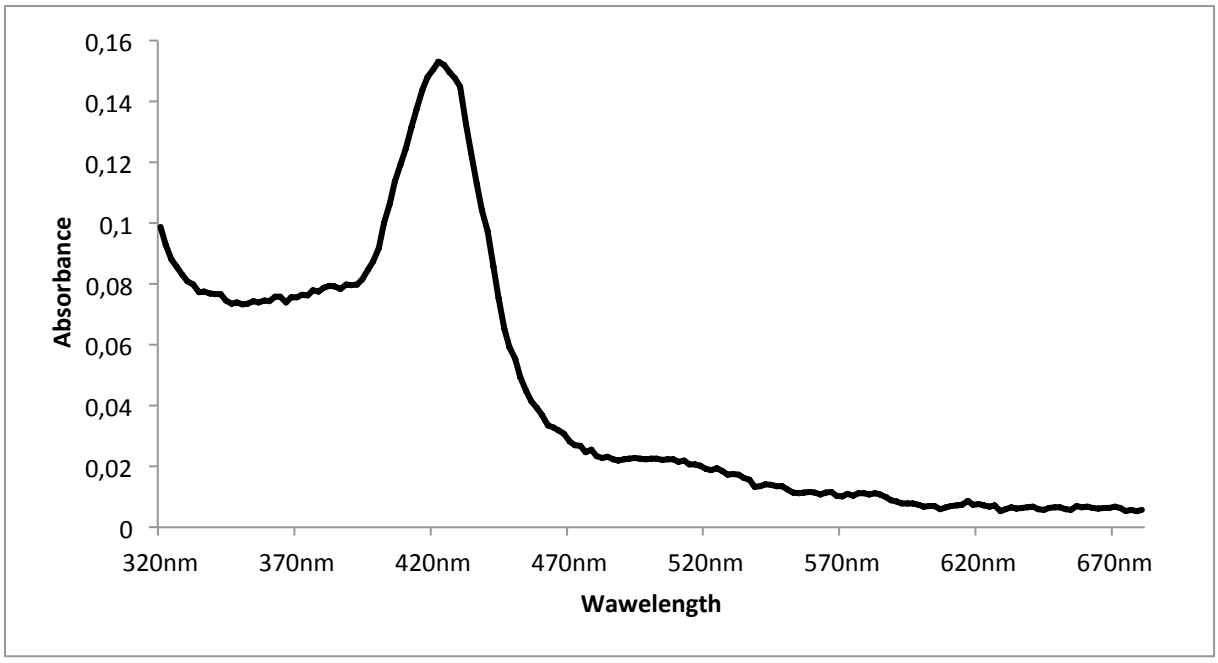
Dendrimer **2e**

λ_{max} (log ε): 423 nm (5.80), 516 nm (4.29), 556 nm (4.14)



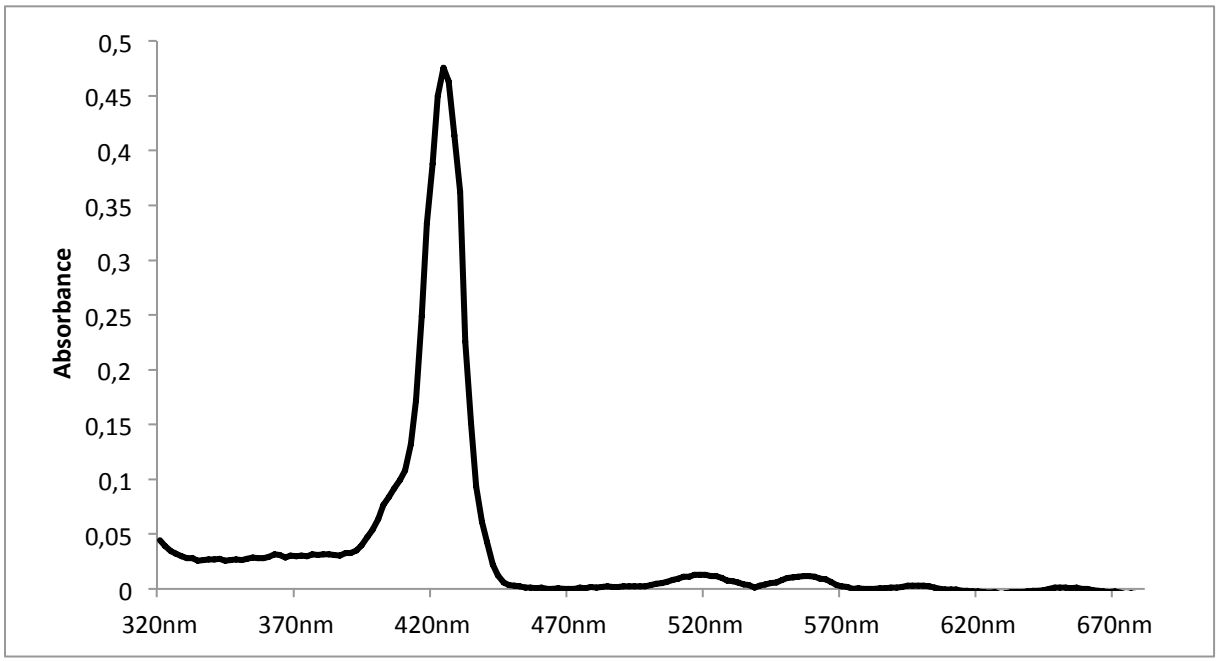
Dendrimer **3e**

λ_{max} (log ε): 422 nm (5.18), 506 nm (4.35), 576 nm (4.05)



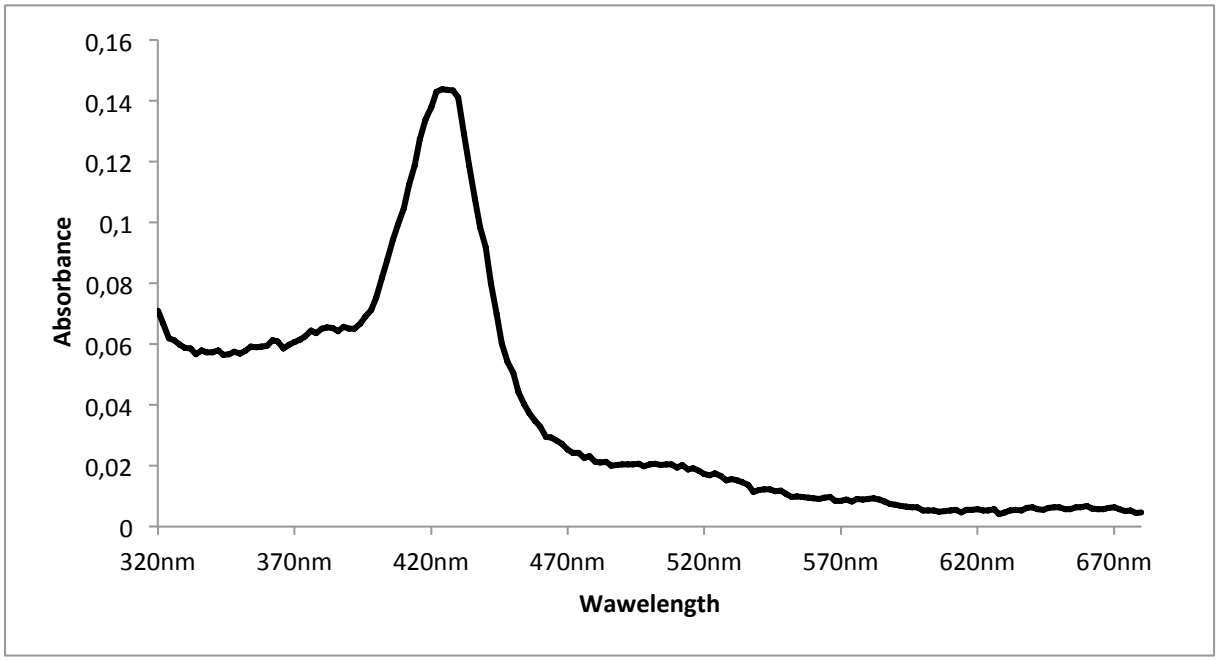
Dendrimer **2f**

λ_{max} (log ε): 425 nm (5.68), 518 nm (4.11), 556 nm (4.08)



Dendrimer **3f**

λ_{max} (log ε): 424 nm (5.16), 508 nm (4.31)



3. Kinetic measurements. ^{1}H NMR data measured for the reaction between 1-chloro-4-(prop-1-en-2-yl)benzene and diazomethane generated *in situ*. Data shown indicate the proportion of the substrate methyl group integral and of the internal standard methyl groups integral against time. The ratio of the integrals before the reaction start (time 0) has been assigned the value of 100. The catalytic experiments were performed according to the procedure described in the Experimental Section of the main text.

Method verification experiments:

Three experiments were performed under identical conditions with **3c** as catalyst, but using different batches of diazomethane precursor **6**. Maximum bias of 5 percent points from the average value at given time was found.

Time (min)	Experiment 1	Experiment 2	Experiment 3
0	100	100	100
20	88	85	81
40	67	64	63
60	50	45	43
80	31	24	27
100	12	5	8
120	5	2	2
140	0	0	0
160	0	0	0

Catalyst amount comparison experiments:

The experiment with 2 mol% of catalyst was run in duplicate.

Time (min)	Amount of catalyst Fe(TPP)Cl (molar %)				
	1%	2% (Exp.1)	2% (Exp. 2)	4%	10%
0	100	100	100	100	100
20	86	78	79	77	84
40	64	58	61	57	67
60	46	39	46	42	54
80	29	24	32	29	48
100	14	11	21	18	44
120	4	4	11	10	39
140	1	1	6	3	31

Catalyst comparison experiments:

Average values from duplicate runs are shown, except for **3f**.

Time (min)	Theoretic ideal progress	Fe(TPP)Cl	3a	3b	3c	3d	3e	3f
0	100	100	100	100	100	100	100	100
20	66	78	83	79	81	80	98	99
40	33	58	66	61	63	61	95	99
60	0	39	47	43	43	40	76	98
80	0	24	29	26	27	20	56	96
100	0	11	14	13	8	4	36	93
120	0	4	4	4	2	1	16	90
140	0	1	1	1	0	0	4	76
160	0	0	0	0	0	0	0	62

Experiment with cease of diazomethane precursor addition:

The addition of solution of **6** was ceased at the time of 60 minutes.

Time (min)	Content of substrate [%]
0	100
20	85
40	68
60	**52**
65	52
70	51
75	51
80	51

4. Cartesian coordinates of dendrimers **2c-f**

2c

246

C	2.93930	-1.00570	-0.26330
C	3.58050	-2.20670	-0.48660
C	2.61190	-3.22740	-0.58920
C	1.35940	-2.67140	-0.43110
N	1.59900	-1.32780	-0.23820
C	3.55380	0.17880	-0.11320
C	0.20620	-3.35690	-0.47000
C	-1.12410	-2.75300	-0.30440
C	-2.31930	-3.43700	-0.29370
C	-3.36670	-2.51280	-0.10070
C	-2.82050	-1.25270	0.00600
N	-1.46030	-1.43090	-0.12320
C	-3.50370	-0.11560	0.20270
C	-2.85320	1.20030	0.32200
C	-3.50120	2.40630	0.47660
C	-2.53310	3.43050	0.57310
C	-1.27870	2.86750	0.47520
N	-1.51310	1.51840	0.32730
C	0.00030	3.59770	0.54660
C	1.19860	3.00550	0.42010
C	2.42110	3.63820	0.48700
C	3.43460	2.67490	0.30610
C	2.84410	1.44570	0.12020
N	1.48920	1.67710	0.19740
C	-4.96860	-0.15000	0.35410
C	0.22960	-4.81430	-0.67510
C	5.02390	0.25680	-0.17590
C	-0.08780	5.05200	0.76000
C	-5.80910	-0.18250	-0.76180
C	-7.19520	-0.23980	-0.60070
C	-7.76620	-0.26850	0.67470
C	-6.92650	-0.22680	1.79240
C	-5.54100	-0.16740	1.62940
C	0.08340	-5.35410	-1.95510

C	0.11470	-6.73590	-2.14480
C	0.29350	-7.59960	-1.06180
C	0.43830	-7.06100	0.22120
C	0.40670	-5.67770	0.41000
C	5.67110	0.57260	-1.37420
C	7.06520	0.62840	-1.43230
C	7.83710	0.37460	-0.29480
C	7.18920	0.06570	0.90640
C	5.79480	0.00590	0.96210
C	-0.46400	5.89570	-0.28820
C	-0.53690	7.27440	-0.09360
C	-0.23500	7.83590	1.14800
C	0.13760	6.99460	2.20220
C	0.20790	5.61240	2.00700
O	-0.32820	9.19620	1.22740
O	-9.13050	-0.34570	0.73580
O	0.31190	-8.93580	-1.34560
O	9.19590	0.43990	-0.44190
C	-0.07440	9.87400	2.44810
C	-9.79610	-0.39820	1.99130
C	0.53430	-9.88680	-0.31450
C	10.03770	0.28140	0.69180
C	-0.23490	11.34760	2.16010
C	-11.27910	-0.53620	1.73160
C	0.50320	-11.24700	-0.96950
C	11.47180	0.33500	0.21990
C	12.01390	1.52190	-0.28820
C	13.34290	1.58630	-0.71400
C	14.13880	0.44030	-0.62970
C	13.62180	-0.75440	-0.12570
C	12.28910	-0.80070	0.29430
C	0.75930	12.04250	1.46150
C	0.63020	13.40360	1.17960
C	-0.51810	14.07880	1.60220
C	-1.52300	13.40710	2.30230
C	-1.37730	12.04270	2.57470
C	-12.05150	-1.46840	2.43430
C	-13.41970	-1.60840	2.19250
C	-14.03240	-0.79830	1.23020
C	-13.28220	0.14650	0.52010
C	-11.91530	0.26970	0.77980
C	-0.69930	-11.95520	-1.07860
C	-0.74860	-13.20170	-1.70410
C	0.42660	-13.74600	-2.22870
C	1.63920	-13.06170	-2.12690
C	1.67120	-11.81350	-1.49740
O	1.66430	13.98600	0.50150
O	-2.60340	14.15120	2.68600
O	-13.79080	0.98020	-0.43820
O	-14.07050	-2.55370	2.93690
O	2.73020	-13.68220	-2.66970
O	-1.97090	-13.81140	-1.76200
O	14.48240	-1.81560	-0.07040
C	1.68150	15.39170	0.29050
C	-3.61220	13.56700	3.49950
C	-15.17730	0.96420	-0.74820
C	-15.43770	-2.86150	2.69920
C	4.02560	-13.11270	-2.54330
C	-2.11980	-15.04710	-2.44750
C	14.07160	-3.05100	0.50000
C	3.02000	15.76600	-0.30220

C	-4.62800	14.64110	3.80490
C	-15.39770	1.95250	-1.86850
C	-15.82560	-3.96780	3.65280
C	4.99690	-14.06990	-3.19320
C	-3.57620	-15.43440	-2.35520
C	15.28410	-3.95100	0.52610
O	13.78210	2.79260	-1.18790
C	15.14200	2.95200	-1.57100
C	15.34010	4.39060	-1.98860
C	3.11180	16.67350	-1.36660
C	4.35400	17.03130	-1.89330
C	5.52250	16.48500	-1.36260
C	5.44550	15.58220	-0.30230
C	4.20300	15.22830	0.22490
C	-5.36980	15.21930	2.76680
C	-6.30230	16.22230	3.03100
C	-6.50820	16.65760	4.33970
C	-5.78220	16.08400	5.38340
C	-4.84880	15.08100	5.11760
C	-15.29400	1.54780	-3.20630
C	-15.49970	2.45750	-4.24420
C	-15.81220	3.78620	-3.95700
C	-15.91380	4.20260	-2.62970
C	-15.70840	3.29110	-1.59290
C	-16.70830	-3.73330	4.71630
C	-17.06300	-4.76350	5.58890
C	-16.53800	-6.04320	5.41000
C	-15.65670	-6.28950	4.35740
C	-15.30470	-5.25860	3.48480
C	5.51130	-13.82220	-4.47340
C	6.40850	-14.71310	-5.06460
C	6.80130	-15.86550	-4.38350
C	6.29320	-16.12520	-3.11080
C	5.39780	-15.23250	-2.52050
C	-4.00700	-16.42400	-1.46120
C	-5.35620	-16.77240	-1.38170
C	-6.29220	-16.13340	-2.19480
C	-5.87590	-15.14610	-3.08770
C	-4.52630	-14.79990	-3.16700
C	15.47200	-4.94980	-0.43900
C	16.60140	-5.76970	-0.40410
C	17.55870	-5.59950	0.59630
C	17.38240	-4.60950	1.56290
C	16.25220	-3.79210	1.52720
C	15.54140	4.73760	-3.33190
C	15.73270	6.06970	-3.70290
C	15.72500	7.07380	-2.73480
C	15.52320	6.74200	-1.39530
C	15.33360	5.40960	-1.02570
H	4.66700	-2.36310	-0.57620
H	2.83740	-4.29010	-0.76880
H	0.83810	-0.62440	-0.08620
H	-2.45190	-4.52270	-0.41090
H	-4.43480	-2.77210	-0.04520
H	-4.58980	2.55910	0.52410
H	-2.75990	4.49860	0.70980
H	-0.74910	0.80920	0.23620
H	2.59850	4.71120	0.65600
H	4.51430	2.88620	0.31210
H	-5.37270	-0.16910	-1.77460
H	-7.84840	-0.26880	-1.48950

H	-7.33630	-0.24440	2.81470
H	-4.88730	-0.14230	2.51730
H	-0.05670	-4.68320	-2.81940
H	-0.00170	-7.15090	-3.16000
H	0.57950	-7.71010	1.09980
H	0.52280	-5.25960	1.42450
H	5.07450	0.77460	-2.27970
H	7.56420	0.87410	-2.38530
H	7.75990	-0.14170	1.82490
H	5.29630	-0.24480	1.91330
H	-0.70000	5.46830	-1.27650
H	-0.83260	7.93090	-0.92880
H	0.38180	7.40210	3.19610
H	0.50130	4.95410	2.84210
H	-0.79070	9.54220	3.22930
H	0.95670	9.66620	2.80490
H	-9.42540	-1.26470	2.57950
H	-9.60440	0.53120	2.56980
H	1.51780	-9.71040	0.17180
H	-0.25860	-9.81150	0.45960
H	9.84960	1.09380	1.42620
H	9.83540	-0.69120	1.18880
H	11.38430	2.42540	-0.35400
H	15.18940	0.45560	-0.95590
H	11.86390	-1.73510	0.69200
H	1.66300	11.50900	1.12300
H	-0.65340	15.15050	1.39430
H	-2.16250	11.49210	3.11490
H	-11.57900	-2.11370	3.19320
H	-15.10760	-0.90250	1.03250
H	-11.33050	1.01680	0.21550
H	-1.62880	-11.52200	-0.67340
H	0.42180	-14.72480	-2.73180
H	2.61480	-11.25170	-1.41660
H	0.85120	15.68080	-0.38850
H	1.55510	15.92990	1.25460
H	-4.10290	12.72560	2.96440
H	-3.16580	13.17610	4.43870
H	-15.49060	-0.05220	-1.06930
H	-15.77540	1.24720	0.14440
H	-16.06950	-1.96300	2.86460
H	-15.58270	-3.20070	1.65070
H	4.06190	-12.12000	-3.04070
H	4.28710	-12.97570	-1.47190
H	-1.82280	-14.93820	-3.51280
H	-1.47880	-15.82730	-1.98400
H	13.69540	-2.89790	1.53430
H	13.25650	-3.50280	-0.10450
H	15.81560	2.71610	-0.71860
H	15.38760	2.26410	-2.40830
H	2.19780	17.11780	-1.79500
H	4.41270	17.74930	-2.72870
H	6.50450	16.76760	-1.77870
H	6.36680	15.14920	0.12260
H	4.15690	14.51750	1.06770
H	-5.21010	14.88550	1.72750
H	-6.87340	16.67280	2.20210
H	-7.24270	17.45350	4.54820
H	-5.94310	16.42600	6.41980
H	-4.27980	14.64060	5.95390
H	-15.04460	0.50080	-3.44760

H	-15.41360	2.12550	-5.29270
H	-15.97540	4.50610	-4.77700
H	-16.15510	5.25400	-2.39910
H	-15.78860	3.63520	-0.54810
H	-17.13100	-2.72680	4.87250
H	-17.75820	-4.56490	6.42180
H	-16.81750	-6.85710	6.10010
H	-15.23600	-7.29950	4.21520
H	-14.60500	-5.46520	2.65690
H	5.20670	-12.91700	-5.02600
H	6.80620	-14.50630	-6.07250
H	7.50900	-16.57040	-4.85160
H	6.59790	-17.03750	-2.57110
H	4.99940	-15.45100	-1.51530
H	-3.27850	-16.93490	-0.80910
H	-5.68210	-17.55270	-0.67300
H	-7.35890	-16.40650	-2.12960
H	-6.61320	-14.63640	-3.73060
H	-4.20880	-14.01430	-3.87350
H	14.72590	-5.09330	-1.23900
H	16.73770	-6.55250	-1.16930
H	18.45250	-6.24520	0.62210
H	18.13670	-4.47180	2.35550
H	16.12640	-3.00960	2.29450
H	15.55040	3.95560	-4.10980
H	15.89070	6.32900	-4.76330
H	15.87640	8.12680	-3.02740
H	15.51400	7.53340	-0.62730
H	15.17410	5.16020	0.03700

2d

470

C	2.75140	-0.80310	-0.38830
C	3.41520	-2.00450	-0.52710
C	2.46540	-3.04350	-0.60920
C	1.20170	-2.49890	-0.51080
N	1.41570	-1.14450	-0.38400
C	3.33990	0.39820	-0.27520
C	0.06150	-3.20490	-0.52130
C	-1.27600	-2.62220	-0.33590
C	-2.45210	-3.33500	-0.27300
C	-3.51410	-2.43320	-0.05810
C	-2.99750	-1.15690	0.00480
N	-1.63840	-1.30530	-0.16600
C	-3.70540	-0.03370	0.20270
C	-3.08770	1.30270	0.26620
C	-3.75860	2.49910	0.39800
C	-2.81370	3.54840	0.42180
C	-1.55020	3.01050	0.30150
N	-1.75670	1.65220	0.21340
C	-0.28540	3.76690	0.28040
C	0.91970	3.19200	0.14220
C	2.12460	3.85980	0.09470
C	3.15730	2.91470	-0.06660
C	2.59750	1.65790	-0.11540
N	1.23990	1.85800	0.00920
C	-5.16610	-0.10430	0.38830
C	0.11320	-4.66860	-0.66640
C	4.81090	0.50270	-0.28340

C	-0.38390	5.22900	0.43010
C	-6.00930	-0.41000	-0.68380
C	-7.38750	-0.51680	-0.49230
C	-7.94970	-0.31900	0.77080
C	-7.11080	0.00040	1.84320
C	-5.73060	0.10540	1.65110
C	0.23860	-5.25610	-1.92810
C	0.28910	-6.64450	-2.05710
C	0.22030	-7.46720	-0.93100
C	0.09910	-6.87970	0.33290
C	0.04570	-5.49070	0.46130
C	5.53910	0.29480	-1.45790
C	6.93250	0.37880	-1.45140
C	7.62430	0.67220	-0.27410
C	6.89640	0.88940	0.90130
C	5.50270	0.80300	0.89370
C	-0.77200	6.03750	-0.64210
C	-0.82450	7.42780	-0.50450
C	-0.48710	8.02940	0.71270
C	-0.11390	7.21960	1.78790
C	-0.06160	5.83220	1.64920
O	-0.48140	9.37790	0.93710
O	-9.30550	-0.46330	0.86360
O	0.27890	-8.81370	-1.15250
O	8.98880	0.71750	-0.35880
C	-0.70730	10.28540	-0.13310
C	-9.97730	-0.26970	2.10130
C	0.28840	-9.71290	-0.05360
C	9.76460	0.95770	0.80650
C	-0.54630	11.68120	0.42290
C	-11.45070	-0.48810	1.84840
C	0.39220	-11.10410	-0.62970
C	11.21740	0.82550	0.41530
C	11.93310	1.92330	-0.07780
C	13.28010	1.80900	-0.42910
C	13.91600	0.57260	-0.29300
C	13.22320	-0.53730	0.19360
C	11.87610	-0.40430	0.54550
C	0.53170	12.49870	0.05890
C	0.67490	13.78600	0.58410
C	-0.28410	14.26630	1.48440
C	-1.36690	13.46580	1.86330
C	-1.48660	12.18160	1.33050
C	-12.17730	-1.47110	2.53140
C	-13.53620	-1.67520	2.27650
C	-14.18250	-0.87860	1.32490
C	-13.47770	0.11370	0.63600
C	-12.12080	0.29990	0.90520
C	-0.73770	-11.92270	-0.74140
C	-0.64710	-13.20800	-1.27830
C	0.59600	-13.67610	-1.71260
C	1.73570	-12.87610	-1.61390
C	1.62840	-11.59330	-1.07100
O	1.77340	14.49930	0.17970
O	-2.34170	13.85030	2.74250
O	-14.02470	0.93510	-0.31030
O	-14.14730	-2.66880	2.99150
O	2.90120	-13.42300	-2.07160
O	-1.80720	-13.92860	-1.34630
O	13.93600	-1.69990	0.29520
C	2.00170	15.80100	0.70520

C	-2.36790	15.17560	3.25410
C	-15.39760	0.82760	-0.66020
C	-15.50540	-3.00470	2.73930
C	4.10800	-12.67250	-2.06130
C	-1.79250	-15.23800	-1.89710
C	13.33460	-2.85790	0.85650
C	3.32100	16.37120	0.23210
C	-3.59130	15.30400	4.13100
C	-15.73620	1.81540	-1.75340
C	-15.93090	-4.17820	3.59320
C	5.23110	-13.49640	-2.65060
C	-3.19140	-15.80890	-1.93660
C	14.33790	-3.98700	0.92170
O	13.89730	2.94000	-0.88630
C	15.30560	2.95930	-1.08440
C	15.74640	4.35780	-1.45440
C	3.72450	17.61740	0.73700
C	4.93590	18.19560	0.34880
C	5.75160	17.51550	-0.55410
C	5.37620	16.27640	-1.07320
C	4.15910	15.71030	-0.67860
C	-4.86460	15.09710	3.58870
C	-6.01290	15.20620	4.37330
C	-5.88530	15.53700	5.72490
C	-4.62640	15.75780	6.28850
C	-3.48510	15.63600	5.48810
C	-17.02340	1.80260	-2.30430
C	-17.38550	2.68110	-3.32690
C	-16.44510	3.59720	-3.80930
C	-15.15400	3.63130	-3.27250
C	-14.81270	2.74360	-2.24990
C	-17.27130	-4.58910	3.56230
C	-17.71120	-5.67420	4.32700
C	-16.79860	-6.35740	5.13190
C	-15.45760	-5.96750	5.18070
C	-15.03640	-4.88170	4.41070
C	6.50380	-12.92420	-2.76870
C	7.57160	-13.63890	-3.31130
C	7.36450	-14.95290	-3.74220
C	6.10300	-15.55680	-3.63590
C	5.04870	-14.81400	-3.08910
C	-3.35280	-17.17940	-2.18050
C	-4.61940	-17.76000	-2.25740
C	-5.74650	-16.95320	-2.08320
C	-5.61470	-15.58610	-1.83050
C	-4.33740	-15.02020	-1.76160
C	13.87190	-5.28450	1.16430
C	14.74610	-6.36860	1.24170
C	16.11660	-6.15220	1.07800
C	16.61100	-4.86660	0.84250
C	15.71750	-3.79160	0.76540
C	16.97860	4.55500	-2.09230
C	17.42100	5.83340	-2.44060
C	16.61370	6.93550	-2.14400
C	15.38430	6.76700	-1.50360
C	14.96030	5.48000	-1.16000
O	5.40090	19.40010	0.79720
O	6.25540	15.70260	-1.94800
O	-18.66590	2.56840	-3.79360
O	-14.16790	4.48410	-3.68550
O	-14.50410	-6.58440	5.94290

O	-18.99970	-6.13180	4.34890
C	5.92190	-16.97870	-4.12260
O	8.76720	-12.97920	-3.38260
O	-6.77890	-14.88660	-1.67020
O	-4.66230	-19.10470	-2.50270
O	17.96830	-4.74940	0.70600
O	14.17200	-7.58450	1.48120
O	14.66470	7.90180	-1.25050
O	18.63970	5.91470	-3.05700
O	-4.60300	16.09070	7.61500
O	-7.20180	14.97890	3.73970
C	6.06500	14.37180	-2.40730
C	7.25910	14.01080	-3.26060
C	4.62700	20.19410	1.68530
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C	-13.07010	6.06020	-5.05510
C	-19.08780	3.31930	-4.92270
C	-20.50740	2.90540	-5.22580
C	-14.84360	-7.72140	6.72460
C	-13.59290	-8.16970	7.44200
C	-19.99650	-5.49980	3.55890
C	-21.29660	-6.22590	3.80760
O	4.62060	-17.45060	-3.79830
C	9.88780	-13.57530	-4.02070
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C	-6.75660	-13.53220	-1.23950
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C	-5.90780	-19.75080	-2.73180
C	-5.64480	-21.21410	-3.00250
C	18.55380	-3.47460	0.47580
C	14.94780	-8.77360	1.46580
C	13.99320	-9.91840	1.70890
C	13.41910	7.81820	-0.57120
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C	8.20660	13.19480	-5.34620
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O	1.17850	-4.86440	-2.93870
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C	6.13660	-8.28920	-5.83650
C	6.65530	-9.55150	-5.52420
C	7.63670	-10.14640	-6.31710
C	8.12290	-9.46310	-7.43680
C	7.62330	-8.19800	-7.76710
C	6.63060	-7.62080	-6.96760
O	8.14380	-7.59670	-8.87990
O	8.04950	-11.38640	-5.92450
C	9.10980	-6.78910	-11.34330
C	9.70590	-6.37820	-12.53680
C	9.57750	-5.06030	-12.96770
C	8.85060	-4.15250	-12.20110
C	8.25450	-4.56160	-11.00630
C	8.37740	-5.88560	-10.56040
C	9.05680	-13.55580	-6.16620
C	9.69140	-14.54830	-6.92660
C	9.88860	-15.82820	-6.40430
C	9.45350	-16.13370	-5.11640
C	8.82120	-15.15660	-4.35120
C	8.62530	-13.87510	-4.86970
C	0.39080	-5.64170	-3.85430
C	-1.08160	-5.65550	-3.46770
C	-1.93870	-6.69170	-3.89730
C	-3.31250	-6.67360	-3.62640
C	-3.82960	-5.64130	-2.84360

C	-2.99610	-4.61690	-2.39470
C	-1.63880	-4.61130	-2.71680
O	-3.60880	-3.65740	-1.65730
O	-4.12380	-7.63930	-4.17750
C	-4.30810	-1.24250	-0.74190
C	-4.32560	-0.77960	-0.11620
C	-5.82960	-0.18740	0.96660
C	-6.85960	-0.25410	0.07590
C	-6.64480	-0.83030	-1.15590
C	-5.48730	-1.44460	-1.67120
C	-6.57340	-9.41490	-5.13740
C	-5.87520	-8.31800	-5.67200
C	-5.55370	-8.33390	-7.04090
C	-5.89160	-9.44670	-7.83180
C	-6.55050	-10.55450	-7.28340
C	-6.90590	-10.52350	-5.93300
C	17.66990	12.63040	2.96800
C	16.66760	13.29790	3.89690
C	15.39960	13.74330	3.48530
C	14.51280	14.34400	4.39720
C	14.92010	14.51220	5.72970
C	16.16570	14.04750	6.16270
C	17.03150	13.44510	5.24320
O	16.45590	14.20580	7.49170
O	13.26990	14.73420	3.94920
C	17.51810	13.42020	8.03850
C	17.56690	13.60180	9.54000
C	18.78510	13.38060	10.19210
C	18.90320	13.50820	11.57570
C	17.77380	13.86480	12.31700
C	16.54310	14.08580	11.69290
C	16.44500	13.95240	10.30350
O	15.49510	14.41910	12.50800
O	20.14100	13.26740	12.11110
C	13.20730	14.96890	13.04500
C	11.94530	15.47080	12.68890
C	10.99890	15.78810	13.66570
C	11.30000	15.60480	15.01480
C	12.54750	15.10300	15.38420
C	13.49270	14.78550	14.40640
C	21.82100	13.16840	13.85890
C	22.23550	13.17750	15.20140
C	23.56890	12.93330	15.54200
C	24.50980	12.67640	14.54710
C	24.11270	12.66630	13.21250
C	22.78220	12.91050	12.87220
C	12.16850	14.77420	4.86720
C	10.84090	14.98230	4.15740
C	9.72260	15.46560	4.85870
C	8.48120	15.62950	4.23710
C	8.33630	15.28620	2.89130
C	9.42950	14.79480	2.18020
C	10.66990	14.64930	2.80740
O	9.26170	14.48250	0.86310
O	7.47340	16.12490	5.01500
C	9.39750	13.58160	-1.80580
C	9.14300	13.22710	-3.13230
C	9.19100	14.19100	-4.13820
C	9.49290	15.51200	-3.81440
C	9.74510	15.86690	-2.48820
C	9.69910	14.90810	-1.46560

C	3.96700	17.22850	5.10340
C	5.25010	16.86800	5.52670
C	5.59600	17.03800	6.87590
C	4.66650	17.56330	7.77550
C	3.39180	17.92100	7.34050
C	3.04360	17.75160	6.00320
C	22.80980	16.25100	0.98640
C	24.05790	16.88500	0.38670
C	23.98600	17.80250	-0.66330
C	25.15170	18.34940	-1.20740
C	26.42210	17.97190	-0.73200
C	26.51290	17.06150	0.32820
C	25.32740	16.53660	0.87220
O	27.75610	16.72680	0.81370
O	24.97540	19.26250	-2.20270
C	27.76500	16.19820	2.15760
C	29.17850	16.22640	2.70360
C	29.74880	15.09780	3.32320
C	31.04670	15.14830	3.84200
C	31.78650	16.33640	3.70810
C	31.24000	17.47650	3.08770
C	29.92140	17.41810	2.61470
O	32.00320	18.62300	2.94550
O	31.49470	14.00450	4.45840
C	31.71360	19.56700	1.78610
C	32.95270	20.48040	1.80350
C	33.01080	21.73270	2.45560
C	34.18670	22.51150	2.46370
C	35.33780	22.05100	1.81490
C	35.29760	20.80830	1.16610
C	34.12270	20.03320	1.15970
C	32.50820	12.82440	6.28310
C	33.62160	12.49370	7.06700
C	33.58580	11.39880	7.93080
C	32.43740	10.61560	8.02280
C	31.32500	10.92930	7.24550
C	31.35770	12.02600	6.38340
C	25.86460	20.37110	-2.16410
C	25.38800	21.40700	-3.15350
C	26.32880	22.07750	-3.94980
C	25.92330	23.02850	-4.89360
C	24.55060	23.28250	-5.03570
C	23.59810	22.64110	-4.23650
C	24.02560	21.70860	-3.28670
O	22.26950	22.92440	-4.44540
O	26.89410	23.65110	-5.65290
C	19.52780	23.65100	-3.46430
C	18.31020	24.29940	-3.70720
C	17.49040	23.89480	-4.76760
C	17.88800	22.83130	-5.58210
C	19.10790	22.18470	-5.33940
C	19.94300	22.58630	-4.28190
C	27.49020	26.05730	-8.51260
C	27.65690	25.01510	-7.57810
C	28.93250	24.45420	-7.43910
C	30.00760	24.92590	-8.18920
C	29.83590	25.96260	-9.09790
C	28.57490	26.52440	-9.26240
O	22.84490	14.84870	0.54450
O	7.26260	0.93350	1.56400
C	8.05580	2.06890	1.93500

C	7.31590	2.94300	2.91770
C	8.07180	3.78740	3.73470
C	7.47370	4.60220	4.69190
C	6.08070	4.57220	4.83540
C	5.30220	3.74540	4.01690
C	5.92450	2.94520	3.05170
O	3.95090	3.75760	4.22270
O	8.33200	5.37290	5.42770
C	3.12890	2.86580	3.47780
C	1.70530	2.92690	3.97910
C	0.76170	2.01680	3.48990
C	-0.56600	2.05490	3.91600
C	-0.94770	3.00610	4.86900
C	-0.02300	3.92570	5.36610
C	1.29850	3.88100	4.91680
O	-0.46300	4.84630	6.27690
O	-1.43170	1.15830	3.34620
C	0.32650	6.01910	6.48980
C	-0.42640	6.99200	7.36730
C	0.27330	7.91390	8.15930
C	-0.41210	8.83370	8.95660
C	-1.80610	8.84520	8.97250
C	-2.51260	7.93660	8.18700
C	-1.82690	7.01990	7.38890
C	-3.96180	-0.80120	3.09690
C	-3.55800	0.46700	2.60470
C	-3.89810	0.46630	1.08860
C	-4.18250	0.08020	0.70860
C	-4.98850	-1.62630	1.15990
C	-4.67210	-1.79220	2.44720
C	7.80520	6.26240	6.39850
C	8.90990	7.05970	7.05780
C	8.50930	7.96550	8.04570
C	9.43180	8.76850	8.70460
C	10.78330	8.65980	8.37660
C	11.21640	7.75820	7.40270
C	10.27670	6.95860	6.74110
O	12.56600	7.75260	7.18460
O	8.92060	9.62070	9.63840
C	13.20050	6.88310	6.25310
C	14.69740	7.13050	6.28100
C	15.55240	6.32370	5.51120
C	16.93710	6.52870	5.51800
C	17.49150	7.54540	6.29600
C	16.65860	8.35580	7.06600
C	15.27610	8.14930	7.05710
C	9.52410	12.01790	12.25410
C	8.93660	11.51660	11.08270
C	7.60370	11.85010	10.79050
C	6.86850	12.66110	11.65960
C	7.46200	13.14920	12.82540
C	8.78880	12.82850	13.12210
O	20.91210	-8.74950	-1.96880
C	20.68260	-9.69780	-0.94090
C	20.80980	-11.05830	-1.55940
C	19.72310	-11.92700	-1.66280
C	19.89760	-13.18350	-2.24640
C	21.16200	-13.54610	-2.75810
C	22.27190	-12.69440	-2.60650
C	22.07500	-11.45330	-1.99750
O	18.79490	-13.99650	-2.23770

C	18.97420	-15.37210	-2.51360
C	17.69680	-16.13360	-2.25200
C	17.75810	-17.52740	-2.36760
C	16.64360	-18.32810	-2.12500
C	15.44470	-17.70940	-1.75180
C	15.34920	-16.31550	-1.64180
C	16.48180	-15.53160	-1.89410
O	14.11880	-15.82220	-1.28720
O	16.79530	-19.68090	-2.27950
C	13.87840	-14.41690	-1.31080
C	12.43160	-14.10560	-0.97650
C	12.06770	-12.78790	-0.66400
C	10.74560	-12.44550	-0.37050
C	9.76370	-13.43840	-0.38350
C	10.09280	-14.76330	-0.68840
C	11.42320	-15.08270	-0.98690
O	9.05720	-15.66040	-0.66860
O	10.51240	-11.13000	-0.09050
C	9.24540	-17.05250	-0.90300
C	7.92880	-17.78550	-0.72290
C	7.86000	-19.17430	-0.93030
C	6.65850	-19.86820	-0.75760
C	5.50340	-19.18700	-0.37440
C	5.55440	-17.80990	-0.16750
C	6.75370	-17.11730	-0.34060
C	8.15130	-8.40860	0.61270
C	9.32540	-9.14170	0.39800
C	10.55350	-8.45980	0.36970
C	10.60160	-7.07890	0.54950
C	9.42450	-6.36140	0.76070
C	8.19910	-7.02800	0.79260
C	15.64900	-20.52670	-2.35230
C	16.01180	-21.92670	-2.81340
C	15.09340	-22.98950	-2.73830
C	15.41550	-24.27570	-3.19070
C	16.68290	-24.50700	-3.73390
C	17.62310	-23.47080	-3.80520
C	17.27920	-22.19370	-3.35110
O	18.83730	-23.80870	-4.33530
O	14.44790	-25.23470	-3.06120
C	19.95840	-22.93150	-4.38480
C	21.05610	-23.72400	-5.06930
C	21.96330	-23.09920	-5.94810
C	22.94240	-23.84750	-6.61380
C	23.02780	-25.22930	-6.40430
C	22.13960	-25.86020	-5.52500
C	21.16380	-25.11450	-4.85660
C	13.20170	-28.68410	-3.40530
C	13.28040	-27.28550	-3.27460
C	12.11650	-26.58780	-2.89460
C	10.92330	-27.26470	-2.63170
C	10.86710	-28.65550	-2.75110
C	12.00640	-29.36280	-3.14690
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C	24.67560	-12.29440	-2.76970
C	25.97280	-13.02840	-3.08750
C	27.19380	-12.32680	-3.20170
C	28.40840	-12.99480	-3.40270
C	28.39000	-14.38860	-3.52700
C	27.19130	-15.11070	-3.47330
C	25.99440	-14.42710	-3.23150

O	27.30770	-16.46310	-3.67480
O	29.55480	-12.23670	-3.45250
C	26.16990	-17.32110	-3.74630
C	26.57850	-18.73940	-4.10840
C	25.88030	-19.80540	-3.53060
C	26.16770	-21.13440	-3.83250
C	27.17840	-21.41890	-4.75310
C	27.89440	-20.37790	-5.35090
C	27.59590	-19.04620	-5.02370
O	28.85580	-20.75110	-6.24430
O	25.40420	-22.05230	-3.17050
C	29.66420	-19.75350	-6.84580
C	30.66740	-20.41770	-7.75570
C	31.38020	-19.61150	-8.65180
C	32.31290	-20.17020	-9.52250
C	32.54440	-21.54540	-9.50770
C	31.84950	-22.35870	-8.61280
C	30.91780	-21.79860	-7.73900
C	24.42080	-24.18340	-2.73010
C	24.54740	-25.57810	-2.69300
C	23.65330	-26.36020	-1.96610
C	22.61260	-25.75550	-1.26140
C	22.46720	-24.36750	-1.29150
C	23.36460	-23.58500	-2.02160
C	30.77390	-12.71880	-4.03010
C	31.79660	-11.59890	-4.12770
C	33.16850	-11.84290	-3.98550
C	34.10280	-10.82320	-4.16310
C	33.67840	-9.52320	-4.44980
C	32.31590	-9.24270	-4.57880
C	31.39410	-10.28800	-4.43160
O	31.99370	-7.93940	-4.86190
O	35.39870	-11.21040	-4.04240
C	30.64530	-7.48420	-4.93690
C	30.61680	-5.96420	-4.98420
C	29.39240	-5.27660	-4.89290
C	29.34750	-3.87800	-4.92480
C	30.52370	-3.13630	-5.04960
C	31.74550	-3.80110	-5.14300
C	31.78920	-5.19730	-5.11080
C	38.77300	-10.32010	-3.68060
C	37.70250	-11.10140	-4.11840
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C	40.14950	-12.29510	-3.48540
C	39.99020	-10.91200	-3.36780
O	29.83780	0.30360	-0.56220
C	30.49140	1.57160	-0.73220
C	31.97880	1.34540	-0.52360
C	32.82600	2.32530	0.03500
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C	34.71960	0.81730	-0.14590
C	33.88040	-0.18240	-0.64420
C	32.53030	0.09750	-0.85750
O	35.01450	3.09440	0.67850
C	36.44830	2.99000	0.58210
C	37.14480	4.32920	0.79180
C	38.48120	4.42250	1.23790
C	39.10250	5.66780	1.40410
C	38.37650	6.83840	1.16990
C	37.05510	6.77770	0.71580

C	36.46180	5.52390	0.49350
O	36.43430	7.98940	0.52810
O	40.41470	5.65230	1.78790
C	35.11370	8.08970	-0.01000
C	34.75190	9.56280	-0.15030
C	33.51800	10.10640	0.25420
C	33.25190	11.48090	0.12760
C	34.21120	12.31180	-0.44400
C	35.42450	11.79560	-0.88990
C	35.68980	10.43090	-0.73230
O	36.26780	12.70100	-1.46340
O	32.08420	12.07700	0.51370
C	37.38610	12.24410	-2.21110
C	37.99830	13.45360	-2.88560
C	39.37080	13.71290	-2.74520
C	39.95000	14.85380	-3.30550
C	39.16130	15.75470	-4.02240
C	37.80100	15.49030	-4.20490
C	37.22230	14.34620	-3.64480
C	29.24350	11.34370	2.73690
C	30.00360	11.89050	1.69230
C	29.35030	12.60670	0.67250
C	27.95780	12.73300	0.68760
C	27.21200	12.15540	1.72120
C	27.85630	11.47070	2.75440
C	41.15870	6.86400	1.92600
C	42.58710	6.50190	2.26520
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O	45.55980	8.41720	3.19000
C	44.13350	2.53070	2.44150
C	45.02070	1.35440	2.78110
C	44.47990	0.20530	3.38140
C	45.31370	-0.84390	3.77810
C	46.69410	-0.75290	3.57910
C	47.23660	0.37850	2.96280
C	46.40660	1.42520	2.55770
C	47.65610	9.55510	3.72710
C	49.01300	9.55450	4.10490
C	49.70620	10.75470	4.25810
C	49.06310	11.96880	4.04010
C	47.72170	11.98040	3.67300
C	47.02150	10.78790	3.51750
O	34.45470	-1.40550	-0.86430
C	33.66330	-2.49930	-1.34130
C	34.54150	-3.73620	-1.31570
C	34.01610	-4.99610	-0.97710
C	34.82290	-6.14620	-0.98910
C	36.18250	-6.01470	-1.29270
C	36.73870	-4.77080	-1.60020
C	35.91020	-3.63630	-1.62630
O	38.08910	-4.79770	-1.85010
O	34.24780	-7.36040	-0.69540
C	38.74000	-3.62940	-2.32720
C	40.14480	-3.95460	-2.77640
C	40.79990	-2.97250	-3.51610
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C	42.75700	-4.34950	-3.73230
C	42.12320	-5.34450	-2.98810
C	40.81920	-5.15100	-2.51900
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O	42.57660	-2.10170	-4.70840
C	42.16690	-7.51970	-2.05830
C	43.15510	-8.63810	-1.88110
C	42.96800	-9.57710	-0.85890
C	43.90530	-10.58970	-0.65960
C	45.03220	-10.66720	-1.48100
C	45.21170	-9.75010	-2.51710
C	44.27300	-8.74320	-2.71910
C	45.61610	-0.67910	-6.18120
C	44.30890	-0.78560	-5.69210
C	43.44520	0.31480	-5.81910
C	43.88800	1.49160	-6.42720
C	45.19380	1.58040	-6.91220
C	46.05790	0.49310	-6.78770
C	34.90630	-8.60120	-0.98360
C	33.95840	-9.75940	-0.72300
C	34.45290	-11.07000	-0.73270
C	33.61520	-12.15580	-0.50120
C	32.25860	-11.94530	-0.23830
C	31.73470	-10.65200	-0.21900
C	32.58760	-9.57170	-0.47250
O	30.39950	-10.55030	0.06470
O	34.21230	-13.37390	-0.58470
C	27.55320	-10.71980	0.07810
C	26.24980	-10.91410	0.54050
C	25.62690	-9.92890	1.30780
C	26.31110	-8.75090	1.61520
C	27.61950	-8.56200	1.16270
C	28.26150	-9.54550	0.38910
C	34.23360	-15.65000	-1.19450
C	33.99270	-16.91210	-0.64170
C	34.69000	-18.02270	-1.10570
C	35.63520	-17.88130	-2.12480
C	35.89990	-16.62280	-2.66910
C	35.20370	-15.50710	-2.20300
C	32.57210	14.05400	5.39850
C	21.27970	21.91960	-3.97930
C	26.48760	24.49430	-6.75030
C	10.00250	15.31350	-0.03830
C	6.17480	16.31130	4.47100
C	20.37230	13.44110	13.50680
C	14.20130	14.63520	11.95480
C	-5.42400	-7.16450	-4.77480
C	-3.07850	-2.33830	-1.53990
C	8.86470	-12.18430	-6.77750
C	7.70500	-6.29600	-9.26780
C	9.75630	10.64780	10.15810
C	-2.84960	1.43530	3.49220
C	14.58960	-26.56560	-3.55290
C	9.21260	-10.63620	0.20280
C	36.44040	-10.35870	-4.46950
C	25.42790	-23.41580	-3.55720
C	46.92680	8.23290	3.54040
C	31.48770	11.59680	1.72280
C	43.94640	-2.10320	-5.05070
C	29.68160	-9.33220	-0.10110
C	33.37840	-14.50860	-0.70460

H	16.72870	-2.34940	-1.11730
H	18.67370	-4.17790	-1.26040
H	23.96780	-4.42480	-0.34030
H	25.78940	-2.41660	0.08580
H	21.72950	-0.54920	0.32120
H	25.37570	2.81110	0.01550
H	23.48680	4.68290	0.63040
H	18.13880	4.66880	0.96860
H	16.34430	2.71990	0.59960
H	20.22680	1.00040	0.26670
H	26.25850	1.62620	2.26400
H	28.67240	1.91600	1.76270
H	28.11330	-1.29100	-2.39240
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H	20.33120	-5.43190	1.18470
H	15.87170	0.60230	-2.01240
H	13.41830	0.19860	-2.14180
H	13.48300	-1.21170	2.02600
H	15.93280	-0.67110	2.14620
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H	21.45080	7.96860	-0.73160
H	20.73910	7.42070	3.54740
H	20.45020	4.98340	3.14960
H	20.92950	9.89850	-0.27820
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H	11.29380	-1.06520	-2.20320
H	9.22280	-2.46200	-1.97500
H	5.98070	-1.11810	0.58810
H	9.74120	1.03890	0.47130
H	23.07330	12.28110	0.08380
H	20.53360	15.27990	1.88890
H	19.35320	11.11410	1.90870
H	4.96980	-2.97440	-0.21020
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H	2.78540	-6.27160	-4.60730
H	6.46640	-4.60940	-3.07810
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H	8.74320	-3.10650	-12.53900
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H	27.35570	18.38780	-1.17060
H	25.37770	15.81150	1.69950
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H	29.17430	14.15530	3.43350
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H	30.71440	20.21150	1.93310
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H	36.26640	22.66480	1.82200
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H	32.41040	9.75530	8.71150
H	30.41290	10.31280	7.31970
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H	1.37870	7.92310	8.15480
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H	-5.69190	-2.31390	0.60480
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H	7.25920	5.68000	7.17530
H	7.09230	6.96710	5.91080
H	7.43900	8.05260	8.30140
H	11.53740	9.28060	8.88490
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H	14.64370	8.80770	7.67820
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H	9.26930	13.21300	14.04230
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H	22.89990	-10.73370	-1.84170
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H	14.54190	-18.30920	-1.53770
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H	11.68300	-16.12100	-1.23920
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H	11.49780	-9.00560	0.20370
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H	9.46240	-5.26580	0.90200
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H	32.86330	-19.52010	-10.22350
H	33.27770	-21.98770	-10.20430
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H	31.88420	-0.69700	-1.26080
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H	36.83890	2.24340	1.31310
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H	36.17430	-18.76620	-2.50820
H	36.65100	-16.50720	-3.46980
H	35.41120	-14.51380	-2.64060
H	32.47930	14.95730	6.05050
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H	6.22020	17.01850	3.61120
H	20.11890	14.48450	13.79700
H	19.71730	12.74770	14.07840
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H	36.40880	-9.39210	-3.92420
H	36.38780	-10.15170	-5.56080
H	25.16590	-23.51650	-4.63230
H	26.44410	-23.83960	-3.39830
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H	31.58720	10.48340	1.81350
H	44.56450	-2.24690	-4.13650
H	44.15590	-2.93210	-5.76250
H	29.67010	-9.03970	-1.17390
H	30.16530	-8.51650	0.47860
H	32.91980	-14.74040	0.28340
H	32.56620	-14.32980	-1.44430

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1814

O	-8.84980	2.62530	0.37530
C	-9.53930	3.18870	1.48420
C	-11.00840	3.28460	1.13830
C	-11.97890	2.81370	2.03550
C	-13.34090	2.90880	1.73540
C	-13.72950	3.47940	0.52400
C	-12.78550	3.94860	-0.38950
C	-11.42650	3.85460	-0.07330
O	-13.28090	4.46690	-1.55270
O	-14.34830	2.47730	2.55250
C	-12.41360	4.80640	-2.62580
C	-14.05890	1.75220	3.73930
C	-13.28900	5.08420	-3.82570
C	-15.38680	1.41280	4.37470
C	-13.39010	6.36370	-4.38840
C	-14.20740	6.59490	-5.50000
C	-14.92850	5.53290	-6.04800
C	-14.85120	4.25200	-5.50100
C	-14.02710	4.03640	-4.39320
C	-15.87870	2.15990	5.45370
C	-17.11320	1.84960	6.03250
C	-17.84900	0.78110	5.52170
C	-17.38700	0.02580	4.44430
C	-16.15180	0.34940	3.87650
O	-14.36800	7.80610	-6.11240
O	-15.61040	3.28560	-6.10060
O	-18.20650	-0.97990	4.01180
O	-17.67180	2.53280	7.07630
C	-15.70680	1.98770	-5.52930
C	-16.69590	1.20630	-6.36160
C	-13.75410	8.97700	-5.59430
C	-14.14780	10.11330	-6.50820

C	-17.88940	-1.76240	2.86710
C	-16.79750	-2.76100	3.17450
C	-17.03850	3.70170	7.57690
C	-17.91250	4.25410	8.67760
C	-18.02930	1.62610	-6.45780
C	-18.95480	0.91160	-7.22540
C	-18.54010	-0.23870	-7.89990
C	-17.21660	-0.67920	-7.81620
C	-16.30800	0.05000	-7.04800
C	-13.51710	10.26940	-7.74910
C	-13.86910	11.31020	-8.60840
C	-14.88380	12.19140	-8.23050
C	-15.51660	12.07080	-6.99120
C	-15.14370	11.02790	-6.13970
C	-16.86170	-3.56030	4.32230
C	-15.87100	-4.50200	4.60620
C	-14.79510	-4.64880	3.72400
C	-14.71000	-3.86320	2.56990
C	-15.71340	-2.92960	2.30390
C	-19.03880	5.02730	8.36850
C	-19.84710	5.55290	9.38100
C	-19.52550	5.29220	10.71470
C	-18.40950	4.51910	11.04640
C	-17.61060	4.00700	10.02240
O	-16.48220	12.93170	-6.53880
O	-13.18680	11.41530	-9.78880
C	-13.14750	12.67920	-10.44330
C	-12.20190	12.58700	-11.61740
C	-16.85230	14.09460	-7.27540
C	-15.66140	14.99450	-7.51960
C	-14.73660	15.24580	-6.49980
C	-13.58790	15.99990	-6.73630
C	-13.36740	16.52860	-8.01050
C	-14.27400	16.29040	-9.04670
C	-15.42270	15.54040	-8.78920
C	-10.95520	11.96420	-11.48480
C	-10.06780	11.88890	-12.56290
C	-10.44070	12.45420	-13.78380
C	-11.67960	13.07700	-13.94340
C	-12.55360	13.14100	-12.85450
O	-13.69220	-3.94170	1.65920
C	-12.64660	-4.88670	1.83960
C	-11.64970	-4.69130	0.72280
C	-10.77000	-3.60290	0.74650
C	-9.82030	-3.41740	-0.25950
C	-9.75700	-4.33160	-1.31540
C	-10.62710	-5.42590	-1.36240
C	-11.56650	-5.59530	-0.34290
O	-16.02910	-5.23130	5.75320
C	-15.06750	-6.22010	6.09230
C	-15.47140	-6.84450	7.40600
C	-15.31310	-6.14030	8.60440
C	-15.63990	-6.71870	9.83210
C	-16.13130	-8.02720	9.86110
C	-16.30000	-8.74950	8.67660
C	-15.97540	-8.14900	7.45880
O	-18.02920	4.22020	12.32550
C	-18.79680	4.68230	13.42800
O	-20.95500	6.32660	9.16710
C	-18.11530	4.19070	14.68340
C	-21.34880	6.71720	7.85790

C	-20.34950	7.66100	7.22680
O	-20.26870	1.26000	-7.37140
C	-20.77380	2.43260	-6.74810
C	-22.23660	2.53290	-7.10910
C	-23.18720	1.74510	-6.44970
C	-24.54320	1.82540	-6.77320
C	-24.95660	2.70990	-7.77540
C	-24.02320	3.50550	-8.44880
C	-22.67220	3.40960	-8.10930
O	-16.73080	-1.79420	-8.43850
C	-17.58800	-2.60780	-9.22680
C	-16.76290	-3.78100	-9.69900
C	-16.18890	-3.79550	-10.97580
C	-15.41240	-4.87370	-11.40510
C	-15.20790	-5.95140	-10.53850
C	-15.76680	-5.95790	-9.25890
C	-16.54540	-4.87190	-8.84800
C	-16.95330	4.82130	15.14740
C	-16.31120	4.37920	16.30810
C	-16.84380	3.29410	17.00550
C	-17.99830	2.64730	16.56220
C	-18.62920	3.10130	15.39950
C	-19.61650	8.57490	7.99570
C	-18.68600	9.43140	7.39960
C	-18.49710	9.37350	6.01840
C	-19.22460	8.48310	5.22760
C	-20.14940	7.63330	5.84020
O	1.63730	9.76790	2.27870
C	2.36890	10.60750	1.39430
C	2.32160	12.02060	1.92750
C	3.48710	12.79110	2.02520
C	3.45170	14.09460	2.52450
C	2.22610	14.63550	2.92080
C	1.04780	13.89450	2.82020
C	1.10500	12.58770	2.32830
O	-0.09420	14.50930	3.25260
O	4.64790	14.75550	2.59840
C	-1.38100	14.10170	2.80660
C	4.76510	15.98060	3.31190
C	-1.61490	14.60200	1.40070
C	4.45480	15.78790	4.77900
C	-1.98340	15.93560	1.18260
C	-2.20060	16.41960	-0.11070
C	-2.03660	15.56280	-1.20070
C	-1.67110	14.22810	-1.00610
C	-1.46760	13.76010	0.29270
C	3.77250	16.77260	5.50230
C	3.45130	16.59440	6.84880
C	3.82190	15.40850	7.49190
C	4.51230	14.41500	6.79020
C	4.82970	14.61610	5.44640
O	-2.52670	17.71730	-0.39160
O	-1.47650	13.32620	-2.01490
O	4.90260	13.22080	7.32770
O	2.77220	17.61680	7.45040
C	-1.78710	13.67150	-3.35780
C	-1.33530	12.52340	-4.22960
C	-3.37570	18.45470	0.47920
C	-4.80680	18.02480	0.25760
C	4.43800	12.82640	8.61030
C	4.92890	11.41620	8.83150

C	2.25770	17.45550	8.76520
C	1.46740	18.69450	9.11170
C	-0.29500	12.69150	-5.15240
C	0.12660	11.62980	-5.95900
C	-0.50440	10.39070	-5.83490
C	-1.54290	10.19760	-4.92160
C	-1.95040	11.27000	-4.12290
C	-5.38360	17.01200	1.03320
C	-6.71900	16.64080	0.84830
C	-7.47400	17.28190	-0.13540
C	-6.92050	18.28970	-0.92900
C	-5.58900	18.65140	-0.72030
C	6.23640	11.17700	9.26950
C	6.70220	9.87160	9.45990
C	5.84580	8.79700	9.20520
C	4.53560	9.01450	8.76920
C	4.08950	10.32410	8.58760
C	0.47030	19.16370	8.24730
C	-0.26690	20.30360	8.56120
C	-0.02180	20.98010	9.75410
C	0.98280	20.54730	10.62230
C	1.71320	19.40160	10.29710
O	-7.59080	18.97320	-1.90430
O	-7.36680	15.68840	1.58720
C	-6.70330	14.98600	2.63100
C	-6.26340	15.90840	3.74460
C	-8.95610	18.69000	-2.17230
C	-9.41070	19.65980	-3.23710
C	-9.26240	19.35550	-4.59580
C	-9.67910	20.25060	-5.58350
C	-10.25040	21.46840	-5.20310
C	-10.40550	21.79610	-3.85480
C	-9.98350	20.88720	-2.88010
C	-5.03990	15.69520	4.38880
C	-4.58220	16.55770	5.38430
C	-5.37840	17.63940	5.77130
C	-6.61380	17.86430	5.15710
C	-7.04460	16.99760	4.14800
O	3.62500	8.02960	8.50740
C	3.99450	6.65750	8.53210
C	2.71660	5.85240	8.48840
C	1.78910	5.99320	9.52910
C	0.60200	5.26180	9.54790
C	0.34450	4.36760	8.50690
C	1.25250	4.20710	7.45770
C	2.43520	4.95390	7.44950
O	7.96960	9.56520	9.87570
C	8.89860	10.61230	10.12500
C	10.25660	10.02720	10.43480
C	10.72170	8.87380	9.78990
C	12.00000	8.37170	10.05080
C	12.82420	9.03440	10.96180
C	12.38080	10.18410	11.62010
C	11.10040	10.66930	11.35010
O	1.31480	21.19230	11.78060
C	0.84340	22.51800	11.98060
O	-1.21610	20.76200	7.69830
C	1.49810	23.05750	13.22890
C	-0.74880	21.73220	6.76670
C	-0.42560	23.01620	7.49660
O	1.13530	11.71980	-6.87930

C	1.84040	12.94400	-7.03380
C	2.88970	12.74490	-8.10140
C	2.53030	12.70310	-9.45500
C	3.50320	12.53570	-10.44670
C	4.84510	12.40750	-10.08000
C	5.22430	12.44450	-8.73540
C	4.24060	12.61220	-7.76040
O	-2.08930	8.94380	-4.87590
C	-3.18290	8.63600	-4.02020
C	-4.44440	9.33650	-4.47100
C	-4.78390	9.40110	-5.82770
C	-5.93780	10.05880	-6.25590
C	-6.76610	10.66560	-5.30700
C	-6.46160	10.59510	-3.94560
C	-5.30340	9.92920	-3.53620
C	0.90930	22.86580	14.48340
C	1.49410	23.37510	15.64380
C	2.69470	24.08340	15.54050
C	3.30380	24.28780	14.29800
C	2.70080	23.76980	13.14940
C	-1.45480	23.81320	8.01310
C	-1.17150	24.98590	8.71810
C	0.15830	25.37210	8.89400
C	1.20290	24.59190	8.39070
C	0.90110	23.42020	7.69380
O	9.09270	-1.13840	1.42390
C	9.60380	-2.09230	2.34540
C	11.07430	-2.26590	2.04660
C	12.02220	-1.41110	2.62250
C	13.38650	-1.57110	2.35920
C	13.80200	-2.59580	1.50680
C	12.87460	-3.45820	0.91600
C	11.51700	-3.28520	1.19450
O	13.19880	-4.48890	0.07630
O	14.37020	-0.78240	2.88980
C	14.53720	-4.71110	-0.35190
C	14.02870	0.24960	3.80360
C	14.97030	-3.64540	-1.33220
C	15.30450	0.91520	4.26130
C	16.17760	-2.95280	-1.16350
C	16.57800	-1.96920	-2.07040
C	15.75690	-1.68310	-3.16270
C	14.56980	-2.38640	-3.37820
C	14.18060	-3.35520	-2.45290
C	15.53840	2.27050	4.00350
C	16.69330	2.90400	4.46280
C	17.64160	2.16460	5.17370
C	17.43650	0.80770	5.43430
C	16.26520	0.19210	4.98010
O	17.77600	-1.34870	-1.83050
O	13.76770	-2.18830	-4.47010
O	18.41770	0.16960	6.14110
O	16.80260	4.23760	4.19020
C	14.31810	-1.50640	-5.59180
C	13.36210	-1.59620	-6.75650
C	18.30420	-0.36750	-2.71860
C	18.61680	-0.96770	-4.07160
C	18.30470	-1.21620	6.43310
C	19.52940	-1.60610	7.22700
C	17.74730	5.03550	4.89240
C	17.36200	6.47720	4.65990

C	12.91560	-0.43700	-7.40410
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C	11.65510	-1.76970	-8.96710
C	12.09530	-2.93980	-8.34320
C	12.94490	-2.84240	-7.24000
C	18.08900	-0.41780	-5.24720
C	18.31520	-1.01100	-6.48980
C	19.12740	-2.14720	-6.56840
C	19.69380	-2.69440	-5.41190
C	19.42610	-2.10490	-4.17480
C	19.60400	-1.31650	8.59600
C	20.73050	-1.67370	9.34350
C	21.78800	-2.32500	8.70750
C	21.73940	-2.62080	7.34460
C	20.60570	-2.25810	6.61060
C	16.07370	6.90990	4.99860
C	15.68280	8.23490	4.79020
C	16.59610	9.13970	4.24670
C	17.89020	8.73270	3.90820
C	18.26130	7.40190	4.11580
O	20.49960	-3.79940	-5.39540
O	17.68800	-0.43370	-7.55980
C	17.64460	-1.11610	-8.80630
C	16.72060	-0.35160	-9.72440
C	20.84680	-4.45540	-6.60700
C	21.77950	-5.59020	-6.25720
C	23.08990	-5.32650	-5.84190
C	23.96980	-6.36110	-5.51790
C	23.52960	-7.68490	-5.61150
C	22.22600	-7.97310	-6.02810
C	21.36160	-6.92320	-6.34470
C	15.55630	-0.94340	-10.22950
C	14.71750	-0.25240	-11.10510
C	15.04520	1.05500	-11.47210
C	16.19370	1.67270	-10.97190
C	17.02630	0.96150	-10.10300
O	22.83050	-3.25610	6.81980
C	22.88500	-3.56240	5.43330
C	24.22150	-4.21360	5.16650
C	25.40570	-3.47880	5.30820
C	26.64990	-4.06830	5.06300
C	26.70640	-5.40720	4.66960
C	25.53750	-6.15940	4.52180
C	24.30440	-5.55460	4.77240
O	20.87970	-1.42860	10.68080
C	19.85830	-0.75840	11.40760
C	20.31300	-0.67760	12.84600
C	20.39870	-1.84210	13.62020
C	20.81120	-1.78880	14.95440
C	21.14030	-0.55250	15.51170
C	21.06460	0.62240	14.76210
C	20.64960	0.55130	13.42910
O	18.84070	9.55940	3.37610
C	18.54830	10.93370	3.16400
O	14.44060	8.72180	5.08490
C	19.78990	11.57530	2.59220
C	13.47600	7.87810	5.69790
C	12.23980	8.70470	5.95740
O	11.60650	0.56430	-9.20900
C	12.09590	1.86500	-8.91420
C	11.51970	2.80700	-9.94520

C	10.13310	2.90960	-10.11460
C	9.58590	3.77720	-11.06470
C	10.44250	4.54980	-11.85080
C	11.82780	4.46550	-11.70180
C	12.35800	3.59410	-10.74540
O	11.75720	-4.19850	-8.75770
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C	10.89070	-5.84340	-10.22000
C	11.69780	-6.47700	-11.17210
C	11.58040	-7.84430	-11.42560
C	10.63860	-8.58920	-10.71000
C	9.82340	-7.98060	-9.75280
C	9.95430	-6.60860	-9.51350
C	20.85440	11.93040	3.42870
C	22.00750	12.52840	2.91780
C	22.09350	12.77370	1.54430
C	21.04490	12.42810	0.68850
C	19.89900	11.82790	1.21910
C	12.33690	9.88840	6.69720
C	11.21120	10.67570	6.94910
C	9.96730	10.25550	6.47300
C	9.84220	9.06580	5.74980
C	10.98350	8.30680	5.48570
O	-1.61880	-7.98700	-1.00160
C	-1.49770	-9.01780	-0.03090
C	-2.01070	-10.29640	-0.64990
C	-3.38930	-10.49320	-0.80050
C	-3.89700	-11.67240	-1.34800
C	-3.00560	-12.66840	-1.75180
C	-1.62720	-12.49380	-1.62000
C	-1.13460	-11.30680	-1.06920
O	-0.85040	-13.53200	-2.05010
O	-5.25760	-11.76260	-1.45330
C	0.56030	-13.40150	-2.15650
C	-5.88690	-12.94020	-1.94270
C	1.07490	-14.70070	-2.73190
C	-5.77360	-14.07800	-0.95270
C	0.58680	-15.16550	-3.96020
C	1.02190	-16.37510	-4.50320
C	1.96930	-17.12910	-3.80510
C	2.47760	-16.68430	-2.58290
C	2.02770	-15.47140	-2.05200
C	-5.96810	-13.85150	0.41620
C	-5.89090	-14.90000	1.33780
C	-5.62560	-16.18990	0.87660
C	-5.42170	-16.44200	-0.48080
C	-5.49880	-15.38140	-1.38940
O	0.47020	-16.75050	-5.69790
O	3.39270	-17.50220	-1.98160
O	-5.16570	-17.73970	-0.82930
O	-6.06200	-14.75240	2.68680
C	4.11280	-17.08050	-0.83110
C	5.06820	-18.19290	-0.46300
C	0.87980	-17.96800	-6.30530
C	0.07180	-18.16850	-7.56020
C	-4.63380	-18.04670	-2.11150
C	-4.43760	-19.54240	-2.21330
C	-6.15730	-13.45010	3.24820
C	-6.26810	-13.59220	4.74780
C	5.86400	-18.79790	-1.44530
C	6.73970	-19.83890	-1.12340

C	6.82910	-20.25920	0.20370
C	6.05660	-19.66760	1.20420
C	5.17420	-18.63820	0.86170
C	0.35590	-17.46180	-8.72650
C	-0.32680	-17.61520	-9.92790
C	-1.36100	-18.55550	-9.94690
C	-1.69600	-19.30250	-8.81160
C	-0.97980	-19.09040	-7.62610
C	-4.00480	-20.30390	-1.12030
C	-3.83910	-21.68760	-1.21910
C	-4.10720	-22.32130	-2.43620
C	-4.53390	-21.58230	-3.54220
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C	-7.36080	-13.05990	5.44160
C	-7.46380	-13.17690	6.82840
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C	-5.35610	-14.38150	6.86530
C	-5.27040	-14.25020	5.47720
O	-2.71400	-20.20210	-8.96750
O	0.08220	-16.84230	-10.97500
C	-0.59240	-16.92960	-12.22090
C	0.10080	-15.98590	-13.17600
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C	-1.90620	-22.12330	-7.73660
C	-1.17300	-22.64710	-8.80890
C	-0.11840	-23.53810	-8.60200
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C	-1.56920	-22.52630	-6.43700
C	1.39550	-16.27410	-13.62860
C	2.05200	-15.41610	-14.51580
C	1.39850	-14.26270	-14.95010
C	0.11000	-13.95170	-14.51390
C	-0.53250	-14.81910	-13.62540
O	-4.82280	-22.12330	-4.76290
C	-5.00880	-23.52520	-4.90730
C	-5.43460	-23.75490	-6.33700
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C	-6.24060	-24.13320	-8.99710
C	-4.98180	-24.58150	-8.58180
C	-4.59120	-24.39110	-7.25490
O	-3.42660	-22.33240	-0.08410
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C	-4.32220	-25.72560	-1.06270
C	-5.45630	-26.50590	-1.29150
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C	-4.31900	-15.28180	8.87940
O	-8.57140	-12.61830	7.40160
C	-5.42250	-16.23000	9.29280
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C	-10.06110	-11.94920	9.09470
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C	5.46830	-19.65930	3.56540
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C	-10.06080	-10.54930	9.11910
C	-11.23410	-9.83370	9.35720
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C	-12.44630	-11.92480	9.58220
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C	1.94630	-2.99550	0.27140
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C	2.72520	-0.92500	0.77880
N	1.35460	-0.92340	0.62150
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C	31.36790	-1.12380	6.86220
C	30.02780	-1.51360	6.84340
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C	12.63880	-14.16760	2.54670
C	11.26560	-14.19810	2.79990
C	9.28760	-14.82950	4.25410
O	-10.97260	23.01100	-3.58760

C	-11.79810	24.80450	-2.28900
C	-13.16550	24.93260	-2.57050
C	-13.76880	26.19040	-2.61060
C	-13.01130	27.33560	-2.37000
C	-11.65010	27.22230	-2.09050
C	-11.04750	25.96410	-2.05070
C	-11.15290	23.44010	-2.24560
O	4.32560	-15.11420	5.22830
C	2.26870	-14.26120	6.02330
C	2.60810	-13.76270	7.28890
C	1.95730	-12.64380	7.81000
C	0.95760	-12.00880	7.07470
C	0.61090	-12.49570	5.81510
C	1.26200	-13.61420	5.29240
C	2.97220	-15.47690	5.46830
O	-24.33610	4.39360	-9.44070
C	-25.68510	5.60450	-10.95430
C	-25.53720	6.96090	-10.63330
C	-25.54100	7.93430	-11.63330
C	-25.69280	7.56280	-12.96890
C	-25.83930	6.21640	-13.30130
C	-25.83530	5.24370	-12.30040
C	-25.68180	4.55790	-9.86580
O	11.84930	-21.93410	-4.50480
C	14.14420	-22.46640	-4.69540
C	14.57170	-22.82850	-3.41050
C	15.85930	-22.51370	-2.97270
C	16.73570	-21.83170	-3.81660
C	16.32190	-21.46470	-5.09670
C	15.03430	-21.78010	-5.53280
C	12.75080	-22.81430	-5.16210
O	7.86000	-23.85870	-6.57730
C	7.56780	-25.57070	-8.17770
C	6.92950	-24.96490	-9.26840
C	5.99630	-25.66850	-10.03030
C	5.68860	-26.99040	-9.71060
C	6.31520	-27.60460	-8.62650
C	7.24850	-26.89920	-7.86480
C	8.57860	-24.80030	-7.36210
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C	-6.28320	-15.94800	13.69550
C	-5.86740	-17.23560	14.06410
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C	-3.84020	-16.34230	15.03230
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C	-5.45790	-14.85940	14.01610
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C	21.71090	-11.59980	-6.15940
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C	19.98670	-13.14610	-5.42060
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C	21.08280	-13.49830	-7.54120
C	21.86010	-12.35860	-7.32850
C	22.55060	-10.36740	-5.92180
O	-7.17480	-19.29870	8.15940
C	-7.19190	-20.85890	6.39160
C	-8.39950	-20.80050	5.68340
C	-9.00730	-21.95810	5.19310
C	-8.41030	-23.20200	5.40760
C	-7.20870	-23.26920	6.11090

C	-6.60310	-22.11270	6.59900
C	-6.54570	-19.60180	6.92150
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C	12.51300	5.17730	8.31860
C	13.47160	4.57940	9.14860
C	14.26070	3.52640	8.68480
C	14.09890	3.05350	7.38370
C	13.14330	3.63310	6.55040
C	12.35480	4.68610	7.01510
C	11.66340	6.32180	8.82000
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C	-15.21810	-14.23660	10.19290
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C	-17.08800	-14.22780	11.74570
C	-15.75070	-13.95250	11.45800
C	-13.77180	-13.92490	9.89190
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C	-11.16760	-6.92570	6.54020
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C	-7.39910	10.37420	-9.59900
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C	18.82010	3.13570	-11.65390
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C	21.14060	2.15820	-12.88660
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C	17.58050	3.67820	-10.98450
O	-2.12130	25.80890	9.25570
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C	-2.60100	23.91150	13.08840
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C	14.55240	11.38670	15.21000
C	15.04860	12.28550	16.15530
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C	16.40690	13.32360	14.45250
C	15.91000	12.42420	13.50780
C	14.43750	10.46690	12.85920
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C	26.68310	-7.74310	-5.95860
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C	27.30570	-7.87780	-8.30580
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C	-2.47190	19.26980	4.81490
C	-2.54680	17.32360	6.44540
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C	-10.46110	-7.44880	-5.49310
C	-9.64070	-6.31290	-3.38120

O	-15.43240	-5.94500	10.94090
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C	-3.93650	9.51180	-11.16670
C	-3.88090	8.15290	-10.96210
C	-5.07540	7.47870	-10.85920
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C	-8.28240	10.55950	-11.32720
O	-8.99790	-2.33190	-0.12810
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C	-6.12950	-3.94360	-1.64030
C	-5.22260	-4.96520	-1.35500
C	-5.00540	-5.35940	-0.03560
C	-5.69360	-4.72590	0.99820
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C	-7.82150	-2.19950	-0.91640
O	13.61460	-0.92440	-11.55320
C	11.62710	-1.30830	-12.77040
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C	10.91250	-3.45450	-13.66130
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C	10.29740	-1.03360	-12.42300
C	12.72650	-0.31450	-12.47960
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H	-13.45270	2.35540	4.41670
H	-12.78060	7.23560	-3.91300
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H	-13.94300	2.98830	-3.92080
H	-15.31240	2.95460	5.81450
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H	-16.01260	2.03620	-4.59570
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H	-18.78920	-2.31280	2.56860
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H	-15.64000	10.93020	-5.18010

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H	2.15930	15.69790	3.33440
H	0.19830	11.97750	2.26240
H	-1.51830	12.98740	2.89920
H	-2.14430	14.55700	3.48980
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H	-2.19050	15.94220	-2.15450
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H	2.33060	13.24160	-6.04840
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H	14.40370	1.62210	-12.16470
H	17.97140	1.43530	-9.69280
H	22.05190	-4.24430	5.15790
H	22.79470	-2.63460	4.82660
H	25.33540	-2.42560	5.62090
H	27.70150	-5.85540	4.48010
H	23.38360	-6.15390	4.65630
H	19.69770	0.18270	11.01690
H	18.96290	-1.28470	11.35020
H	20.13450	-2.79750	13.15830
H	21.46980	-0.50270	16.57390
H	20.58630	1.46720	12.81510
H	17.69670	11.04440	2.46540
H	18.27390	11.43260	4.13900
H	13.24170	7.02060	5.03210
H	13.86440	7.48420	6.66400
H	11.79530	2.16580	-7.93560
H	13.20600	1.87410	-8.95870
H	9.43990	2.24800	-9.44040

H	10.04170	5.19830	-12.56020
H	13.46900	3.51530	-10.60240
H	10.03520	-3.91030	-9.87220
H	11.54040	-3.87960	-10.78820
H	12.45410	-5.88210	-11.74600
H	10.52010	-9.66510	-10.88340
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H	20.78710	11.73220	4.52660
H	22.99290	13.24650	1.10550
H	19.06870	11.54730	0.56580
H	13.32930	10.19230	7.07220
H	9.08540	10.88660	6.68310
H	10.88160	7.37570	4.90720
H	-0.43220	-9.12790	0.28190
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H	-7.04000	-12.92760	2.84510
H	5.77630	-18.43070	-2.51100
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H	13.89700	-23.35590	-2.74640
H	16.17280	-22.79340	-1.99280
H	17.75940	-21.58000	-3.46990
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H	14.71550	-21.47600	-6.56300
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H	12.66690	-22.70110	-6.25750
H	7.16890	-23.88730	-9.53710
H	5.50950	-25.18890	-10.86860
H	4.97200	-27.53040	-10.29610
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H	-6.50230	-18.11200	13.82980
H	-4.31220	-18.53420	15.02820
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H	-3.55790	-14.13020	14.94160
H	-5.75740	-13.85530	13.75410
H	-7.64920	-14.77200	12.51460
H	-8.38360	-15.72800	13.71760
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H	14.72800	2.21910	7.01400
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H	-10.24390	-10.70580	-6.49700
H	-11.12460	-8.50270	-7.26670
H	-10.85820	-6.48110	-5.84570
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H	-13.19400	-6.99500	11.64460
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H	-6.28790	-3.63880	-2.69950

H	-4.67160	-5.46140	-2.17440
H	-4.28680	-6.16120	0.18840
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H	-7.13490	-3.21370	1.53700
H	-8.08880	-2.15570	-2.00340
H	-7.34530	-1.21560	-0.67320
H	12.97070	-2.76580	-13.67710
H	11.15780	-4.41070	-14.14830
H	8.79310	-3.90770	-13.51510
H	8.23580	-1.73180	-12.40430
H	10.04450	-0.09330	-11.93790
H	12.31540	0.60490	-12.06180
H	13.25380	-0.06440	-13.40710