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Gas-Phase Synthesis of Racemic Helicenes and their Potential Role in the Enantiomeric Enrichment of Sugars and Amino Acids in Meteorites

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Abstract

The molecular origins of homochirality on Earth is not understood well, particularly how enantiomerically enriched molecules of astrobiological significance like sugars and amino acids might have been synthesized on icy grains in space preceding their delivery to Earth. Polycyclic aromatic hydrocarbons (PAHs) identified in carbonaceous chondrites could have been processed in molecular clouds by circularly polarized light prior to the depletion of enantiomerically enriched helicenes onto carbonaceous grains resulting in chiral islands. However, the fundamental low temperature reaction mechanisms leading to racemic helicenes are still unknown. Here, by exploiting synchrotron based molecular beam photoionization mass spectrometry combined with electronic structure calculations, we provide compelling testimony on barrierless, low temperature pathways leading to racemates of [5] and [6]helicene. Astrochemical modeling advocates that gas-phase reactions in molecular clouds lead to racemates of helicenes suggesting a pathway for future astronomical observation and providing a fundamental understanding for the origin of homochirality on early Earth.

Introduction

The origin of biological homochirality – nature's selection of one specific enantiomer over the other – has remained a highly controversial topic[1-5] since its discovery by Louis Pasteur in 1848. Chiral molecules exist in two mirror images which are not superimposable. On Earth, living organisms developed a strict homochirality with D-sugars and L-amino acids incorporated in ribonucleic acids and polypeptides, respectively.[6] Prevalent routes to homochirality implicate the propagation and amplification of primordial enantiomeric excesses such as the identification of D-enriched sugar alcohols and sugar acids like arabinonic acid[7] along with L-enriched amino acids isovaline, α-methyl norvaline, α-methyl valine, and α-methyl norleucine in the Murchison and Murray meteorites.[8-10] These pathways might be initiated from racemic mixtures of chiral organic molecules like amino acids,[11-15] sugars,[16] and epoxides[17] synthesized in the interstellar medium on ice-coated nanoparticles (interstellar grains) within molecular clouds, of which one enantiomer is preferentially destroyed through asymmetric beta-decay-related radiolysis[18,19] or photolytically by ultraviolet circularly polarized light in star formation regions.[20-23] Magnetars – white dwarfs with magnetic fields exceeding 10^{13} Tesla - may separate racemic mixtures of organic radicals;[24] these paramagnetic radicals may end up in spatially separated sections of the molecular clouds.[24,25] If a primordial enantiomeric excess existed in the molecular cloud, this excess could be passed on via star forming regions to its descendants (planets, moons, comets, meteorites) leading to the homochirality of life on Earth as we know it. Compelling evidence for the delivery of enantiomerically enriched organics from meteorites such as Murchison and Murray to Earth exists,[8,9] however, the question, how did D-sugars and L-amino acids outnumber L-sugars and D-amino acids is still unanswered. A fundamental understanding of the underlying pathways at the molecular, microscopic level is required to answer this question.

Here, molecular beam experiments with isomer-selective photoionization via a targeted, vinylacetylene-mediated gas-phase reaction of aromatic helicenyl radicals coupled with electronic structure calculations and astrochemical modeling reveal an elegant synthetic route to racemic helicenes - ortho-fused polycyclic aromatic hydrocarbons (PAHs),[26] in which benzene building blocks form helically-shaped molecules.[27] The simplest helicenes serve as benchmarks to unravel the exotic gas-phase chemistries leading to a facile low temperature formation of the 22- and 26-π-electron aromatic molecules [5]helicene ($C_{22}H_{14}$) and [6]helicene ($C_{26}H_{16}$) plus atomic hydrogen (1 amu) (reactions (1) and (2)), respectively. Combined with electronic structure calculations and astrochemical modeling, a molecular picture to barrierless, low temperature molecular mass growth processes of helicenes in cold molecular clouds such as TMC-1 and OMC-1 emerges through a stepwise ring annulation one ring at a time via bimolecular gas-phase reactions of an aromatic helicenyl radical with vinylacetylene. These processes were previously conjectured to operate only at elevated temperatures of a few 1,000 K prevailing in circumstellar envelopes of carbon rich stars and planetary nebulae as their descendants since entrance barriers equivalent to a few 100 K prohibit these reactions in cold molecular clouds.[28] Accounting for the handedness of the helix, clockwise and counterclockwise helices are non-superimposable causing an axial chirality (helical chirality) with left- and right-handed helices defined by *minus* (**M**) and *plus* (**P**) (Figure 1).[29] Although the gas-phase mechanism unraveled here leads to *racemates* of [5] and [6]helicenes, i.e. mixtures of equal quantities of the **M** and **P** enantiomers, circularly polarized ultraviolet light[30] as detected toward the Orion Massive Star Forming Region[31] may preferentially photolyze the **M** or **P** enantiomer in the gas-phase of the interstellar medium. This process may initiate the complex chain of reactions ultimately leading to an enantiomeric excess in biorelevant molecules such as D-sugars and L-amino acids and possibly homochirality in our Solar System (Figure 1).

(1) $C_{18}H_{11}^{\bullet}$ (227 amu) + C_4H_4 (52 amu) → $C_{22}H_{14}$ (278 amu) + $H^{\bullet}$ (1 amu)

(2) $C_{22}H_{13}$ (277 amu) + C_4H_4 (52 amu) → $C_{26}H_{16}$ (278 amu) + $H^{\bullet}$ (1 amu)

Experimental

The experiments were carried out at the Chemical Dynamics Beamline (9.0.2) of the Advanced Light Source (ALS) with a resistively-heated silicon carbide (SiC) chemical reactor interfaced to a molecular beam apparatus operated with a Wiley-McLaren reflectron time-of-flight mass spectrometer (Re-TOF-MS).[32] 2-bromobenzo[c]phenanthrene and 9-bromodibenzo[c,g] phenanthrene were synthesized following literature procedures. The [4]helicenyl radicals were prepared *in situ* via pyrolysis of the corresponding brominated precursors. Note that the low vapor pressure of the heated [5]helicenyl precursor prohibited the collection of data at an adequate signal-to-noise ration. Therefore, only a computational study was conducted for this system. The reactants were seeded at a level of less than 0.01 % in a vinylacetylene (5 %) – helium (95 %) carrier gas at 150 Torr and introduced into a resistively heated silicon carbide tube (SiC) with the temperature of 1,585 ± 85 monitored using a Type-C thermocouple. The products formed in the reactor were expanded supersonically and passed through a 2 mm diameter skimmer located 10 mm downstream of the pyrolytic reactor and enter into the main chamber, which houses the Re-TOF-MS. The quasi-continuous tunable vacuum ultraviolet (VUV) light from the Advanced Light Source intercepted the neutral supersonic molecular beam perpendicularly in the extraction region of Re-TOF-MS. VUV single photon ionization is essentially a fragment-free ionization technique and hence is characterized as a *soft ionization* method.[33] The ions formed via photoionization are extracted and detected by a multichannel plate detector. Photoionization efficiency (PIE) curves, which report ion counts as a function of photon energy ranged from 7.00 to 9.50 eV, with a step interval of 0.05 eV at a well-defined mass-to-charge ratio (*m/z*), were produced by integrating the signal recorded at the specific *m/z* for the species of interest.

Theoretical Calculations. The geometric structures, vibrational frequencies, and energies of the local minima and transition states involved in the reactions of [4] and [5]helicenyl radicals with vinylacetylene were computed at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory.[34-36] This dual-level computational approach involves geometry optimization and vibrational frequencies calculations at the density functional B3LYP level of theory with the 6-311G(d,p) basis set. Then, single-point energies of the optimized structures were refined within the framework of the G3(MP2,CC) model chemistry where the total energy of each species is computed as

$$E_0[G3(MP2,CC)] = E[CCSD(T)/6\text{-}31G(d)] + \Delta E_{MP2} + E(ZPE),$$

where ΔE_{MP2} is a basis set correction, ΔE_{MP2} = E[MP2/G3Large] – E[MP2/6-31G(d)], and E(ZPE) is the zero-point energy. Restricted RHF-RCCSD(T) and RMP2 energies were used for open-shell species; RHF-RCCSD(T) stands for partially spin-adapted open-shell coupled cluster singles and doubles theory augmented with a perturbation correction for triple excitations starting from molecular orbitals obtained from restricted open shell Hartree−Fock calculations. For coupled cluster calculations, the degree of a multireference character of wave functions was monitored through T1 diagnostics. The theoretical method used is normally capable to provide a chemical accuracy of 3–6 kJ mol^{-1} for the relative energies and 0.01–0.02 Å for bond lengths as well as 1–2° for bond angles.[37] The GAUSSIAN 09[38] and MOLPRO 2021[39] program packages were used for the B3LYP and G3(MP2,CC) calculations, respectively. – The Rice-Ramsperger-Kassel-Marcus (RRKM) theory,[37,40,41] was used for the calculations of energy-dependent rate constants of all unimolecular steps in the [4]helicenyl + C_4H_4 and [5]helicenyl + C_4H_4 following the formation of the initial intermediates **[i3]** and **[i12]**, respectively, at zero collision energy and in the limit of zero pressure corresponding to the conditions in cold molecular clouds. Note that under such conditions, only **[i3]** can be produced in the [4]helicenyl + C_4H_4 reaction where the vinylacetylene moiety adds to the radical site in the aromatic ring by its vinylic end. Alternatively, in the [5]helicenyl + C_4H_4 reaction, both additions by the vinylic

and acetylenic ends feature submerged barriers and hence RRKM calculations began from the van-der-Waals complex **[i12]**. The computed rate constants were utilized to evaluate product branching ratios under cold molecular clouds conditions within steady-state approximation.[42]

Astrochemical Models. To study the chemistry of PAHs containing up to six six-membered rings in the cold molecular cloud TMC-1, we built the chemical model by expanding the RATE12 network [43] with barrierless neutral – neutral reactions leading to PAHs and their precursors. First, a fiducial time-dependent gas-phase model was operated [43] until the chemistry evolves to steady-state, i.e. after typically 10^7 years. The molecular abundances at this point are then employed as the initial conditions for the next step. Second, the simulations were conducted over multiple runs with the ice mantle species injected into the gas phase through reactive desorption until it reaches the steady state; this strategy was exploited successfully to demonstrate the key role of neutral- neutral reactions in the formation of benzene in TMC-1.[44] These results were then benchmarked with astronomical observations for cyanobenzene (C_6H_5CN), and 1- and 2-cyanonapthalene ($C_{10}H_8CN$) to verify the predictive capabilities of the chemical network (†ESI).

Results & Discussion

Molecular Beams Experiments – Identification of the Molecular Formula of the Product. A chemical micro reactor was utilized to prepare [5]helicene via the gas phase reaction of the benzo[*c*]phenanthren-2-yl radical ($C_{18}H_{11}^{\bullet}$) with vinylacetylene (C_4H_4) (Figure 2a inset). The reaction products were probed isomer-specifically in a molecular beam via tunable vacuum ultraviolet (VUV) light followed by detection of the ionized molecules in a reflectron time-of-flight mass spectrometer (Re-TOF-MS) (Methods). An illustrative mass spectrum recorded at a photoionization energy of 9.50 eV for the reaction of the benzo[*c*]phenanthren-2-yl radical ($C_{18}H_{11}^{\bullet}$) with vinylacetylene (C_4H_4) is shown in

Figure 2 b; reference data were also collected by replacing the vinylacetylene reactant with non-reactive helium carrier gas (Figure 2 a). A detailed comparison of these data reveals compelling evidence for the preparation of a molecule with the molecular formula $C_{22}H_{14}$ (278 amu) along with its ^{13}C counterpart $^{13}CC_{21}H_{14}$ (279 amu) in the benzo[*c*]phenanthren-2-yl – vinylacetylene system (Figure 2b, inset). Considering the molecular weight of the reactants and of the products, the $C_{22}H_{14}$ isomer(s) along with a light hydrogen atom represents the outcome of the reaction of the benzo[*c*]phenanthren-2-yl radical ($C_{18}H_{11}^{\bullet}$; 227 amu) with vinylacetylene (C_4H_4; 52 amu) (reaction (1)). Additional ion counts from *m*/*z* = 226 to 229 and 306–309 are observed in both the benzo[*c*]phenanthren-2-yl – vinylacetylene system *and* in the control experiment; this finding suggests that the generation of these species does not require molecular mass growth processes through the reaction of the benzo[*c*]phenanthren-2-yl radical with vinylacetylene (†ESI; Figure S1).

Molecular Beams Experiments – Identification of the Structural Isomers of the Products. The nature of the structural isomer(s) at *m/z* of 278 ($C_{22}H_{14}^{+}$) prepared in the reaction of the benzo[*c*]phenanthren-2-yl radical with vinylacetylene is revealed by the detailed examination of the corresponding photoionization efficiency (PIE) curve, which portrays the intensity of the ion as a function of the photon energy from 7.00 eV to 9.50 eV (Figure 3a). The experimental PIE curve at *m*/*z* = 278 (Figure 3, black line) can only be fit with a linear combination of known reference PIE curves of distinct isomers of $C_{22}H_{14}$ such as [5]helicene (Figure 3, green line) and benzo[a]tetraphene (Figure 3, blue line). The experimental and reference PIE curves for [5]helicene reveal an onset of the ion signal at 7.40 ± 0.05 eV. However, the PIE curve of [5]helicene alone cannot replicate the ion counts beyond 8.50 eV. Considering the error bars, the contribution of benzo[*a*]tetraphene is clearly required to account for the lack of ion counts from the range of 7.00 eV to 8.50 eV. The overall fit (red) consists of ion counts of [5]helicene (82 ± 5 %) and of benzo[*a*]tetraphene (18 ± 4 %). It is important to note that the actual branching ratios of

[5]helicene versus benzo[*a*]tetraphene require the knowledge of their photoionization cross sections; these are unknown. Electronic structure theory has not advanced to such a level to accurately compute the photoionization cross sections of organic molecules as complex as [5]helicene and benzo[*a*] tetraphene. Nevertheless, our experiments reveal the proof-of-concept that the reaction of benzo[*c*] phenanthren-2-yl radical with vinylacetylene leads to two distinct product isomers via molecular mass growth processes: benzo[*a*]tetraphene (**p1**) and [5]helicene (**p2**). It is critical to highlight that the PIE curve recorded at $m/z = 279$ (Figure 3b) can be associated with ^{13}C substituted isomer ($C_{17}{}^{13}CH_{12}$) of [5]helicene and benzo[*a*]tetraphene with an overall ion count intensities of 22 ± 2 % as predicted from the 1.1 % ^{13}C natural abundance along with 22 carbon atoms in the products.

Electronic Structure Calculations – [5]Helicene and its Isomers. With the experimental determination of distinct isomers [5]helicene and benzo[*a*]tetraphene ($C_{22}H_{14}$), we turn to electronic structure calculations to decipher the pathways that lead to their formation across complex potential energy surfaces. The computations were carried out at the G3(MP2,CC)//B3LYP/6–311G(d,p) level of theory and reveal that the [4]helicenyl radical may approach the vinylacetylene reactant barrierlessly resulting in the formation of two possible van-der-Waals complexes [**i1**] and [**i2**] (Figure 4; Table S1). These complexes are stabilized by 9 and 14 kJ mol^{-1} with respect to the separated reactants and reveal a carbon-carbon distance between the radical center of the benzo[*c*]phenanthren-2-yl radical with the vinyl (C1) and acetylenic (C4) carbon atoms of vinylacetylene of 409 and 388 pm, respectively. The van-der-Waals complexes can isomerize through addition of the radical center to the vinyl (C1) and acetylenic (C4) moieties via barriers of 3 and 16 kJ mol^{-1} yielding intermediates [**i3**] and [**i4**], respectively. A key feature of the addition to the C1 carbon atom is that the transition state to addition lies 6 kJ mol^{-1} *below* the energy of the separated reactants. Therefore, an addition barrier exists, but is lower in energy than the separated reactants and hence is termed a submerged barrier.[45] Whereas [**i3**] and [**i4**] may

undergo unimolecular decomposition via atomic hydrogen loss to 2-((*E*)-but-1-en-3-ynyl)[4] helicene (**p3**) and 2-(but-3-en-1-ynyl)[4]helicene (**p4**), respectively, the resonantly stabilized doublet radical intermediate [**i3**] is fundamental in the formation of [5]helicene (**p2**) and benzo[*a*]tetraphene (**p1**). Benzo[*a*]tetraphene (**p1**) can be accessed via the reaction sequence [**i3**] → [**i5**] → [**i6**] → [**i7**] → **p1** + H, whereas [5]helicene (**p2**) can be prepared via [**i3**] → [**i8**] → [**i9**]/[**i10**] → [**i11**] → **p2** + H involving hydrogen atom shifts and a six-membered ring closure terminated by hydrogen atom losses from the methylene (CH_2) moieties in [**i7**] and [**i11**] through tight transition states located 19 and 20 kJ mol^{-1} above the energy of the separated products in overall exoergic reactions (Δ_RG (**p1**+H) = – 262 kJ mol^{-1}; Δ_RG (**p2**+H) = – 261 kJ mol^{-1}). A detailed analysis of the barriers of isomerization of [**i3**] suggests that [5]helicene (**p2**) is formed preferentially. This deduction gains full support from the theoretically predicted branching ratios of 0.002 % : 99.8 % : 0.2 % for **p3** versus **p2** versus **p1** for cold molecular clouds conditions at 10 K and nearly zero pressure thus amplifying the synthetic route to [5]helicene (**p2**) in low temperature conditions of deep space (10 K). The presence of the submerged barrier is critical since these low temperatures effectively block reactions proceeding via transitions states located above the energy of the separated reactants such as the isomerization of **[i2]** to **[i4]** thus inhibiting the formation of 2-(but-3-en-1-ynyl)[4]helicene (**p4**). Recall that the thermodynamically less stable isomer **p3** was not detected in our study. Consequently, isomerization of [**i3**] and formation of [5]helicene (**p2**) and benzo[*a*]tetraphene (**p1**) is preferred at the expense of unimolecular decomposition to 2-((*E*)-but-1-en-3-ynyl)[4]helicene (**p3**). It is interesting to note that in case of a chiral [4]helicenyl reactant, its reaction with vinylacetylene should form a racemic mixture of [5]helicene. The memory of a particular chirality of the reactant is lost in the intermediate **[i8]**, which exhibits a planar geometry of the four aromatic rings due to the absence of an H atom at the most crowded position on one of the terminal rings. **[i8]** is still chiral due the presence of the CH_2CH_2CCH side chain but it can easily interconvert to its other enantiomer by facile

rotation around the out-of-ring single C–CH_2 bond. Therefore, two different enantiomers of **[i11]** are predicted to be formed in nearly equal amounts and these enantiomers, after losing a hydrogen atom, would give rise to a racemic mixture of the product [5]helicene (**p2**). Alternatively, the particular chirality of the reactant is preserved along the entire reaction pathway toward **p1**; here, the chirality of benzo[*a*]tetraphene will coincide with that of the [4]helicenyl reactant.

Electronic Structure Calculations – [6]Helicene and its Isomers. The concept of a *de-facto* barrierless, vinylacetylene-mediated ring annulation to [4]helicenyl radicals leading to [5]helicene through resonantly stabilized free radical intermediates can be exported to [6]helicene. This mechanism provides a unified and versatile synthetic route to racemic helicenes via successive molecular mass growth processes through bimolecular gas-phase reactions one ring at a time. The key features of the [5]helicenyl – vinylacetylene PES (Figure 5; Table S1) fundamentally mirror the [4]helicenyl – vinylacetylene system (Figure 4). The reaction is initiated through the formation of a van-der-Waals complex [**i12**]. Although two distinct long-range complexes could be located in the [4]-helicenyl-vinylacetylene system, despite an extensive search, only a single van-der-Waals complex was characterized in the reaction of [5]helicenyl with vinylacetylene with distances of at least 400 pm between the radical center and the vinyl and acetylene functional groups. This complex can isomerize through addition of the radical center of [5]helicenyl to the acetylenic or vinyl functional group forming [**i13**] or the resonantly stabilized free radical intermediate [**i14**], respectively. In both cases, the barriers to addition are located below the energy of the separated reactants; therefore, these can be once again be classified as submerged barriers. While [**i13**] may fragment via atomic hydrogen loss to 2-(but-3-en-1-ynyl)[5]helicene (**p5**), the chemistry of [**i14**] is more diverse. This intermediate either eliminates a hydrogen atom to form 2-((*E*)-but-1-en-3-ynyl)[5]helicene (**p6**) or undergoes hydrogen migration from the ortho or para position with respect to the side chain added to

the benzene moiety yielding [**i15**] and [**i16**], respectively. These structures isomerize via ring closure to [**i17**] and [**i18**] followed by another hydrogen migration from the methylene group (CH_2) neighboring the carbene carbon atom to the latter; these shifts form intermediates [**i19**] and [**i20**], when then undergo hydrogen loss from the remaining methylene functional group accompanied by aromatization to [6]helicene (**p7**) and naphtho[1,2-a]tetraphene (**p8**) in overall exoergic reactions ($\Delta_R G$ (**p7**+H) = – 269 kJ mol^{-1}; $\Delta_R G$ (**p8**+H) = – 263 kJ mol^{-1}). The energies of the transition states for isomerization (or fragmentation) of [**i4**] along with the location of the barriers of the subsequent isomerization processes as discussed above advocate a favorable yield of [6]helicene (**p7**). Indeed, the computed branching ratios of 9.0 % : 0.04 % : 87.5 % : 3.4 % for **p5** versus **p6** versus **p7** versus **p8** for cold molecular clouds (10 K) are in line with our hypothesis. The chirality of the [5]-helicenyl reactant is maintained along all reaction pathways and hence will be the same in particular for the [6]helicene (**p7**) and naphto[1,2-*a*]tetraphene (**p8**) products.

Astrochemical Modeling. Having provided compelling evidence on the formation of [5] and [6]helicene through *barrierless* reactions of the helicenyl radicals with vinylacetylene (reactions (1) and (2)), we are applying these findings now to 'real' cold molecular clouds. It is important to highlight that both reactions have no entrance barriers, all barriers involved in the isomerization processes are below the energy of the separates reactants, and the overall reactions (1) and (2) to [5] and [6]helicene are exoergic. These findings denote key requirements for both reactions to proceed in low-temperature environments such as in molecular clouds (10 K). Any barrier located above the energy of the separated reactants would inhibit the reactions to [5] and [6]helicene in molecular clouds; likewise, the low temperatures of the molecular would prohibit endoergic reactions. In this context it is important to emphasize that although the reaction of the 4-phenanthrenyl radical ($C_{14}H_9^{\bullet}$) with vinylacetylene yields [4]helicene ($C_{18}H_{12}$),[28] the inherent barrier to addition

in the entrance channel of 9 kJ mol^{-1} – equivalent to about 800 K – cannot be overcome in cold molecular clouds. This barrier is essentially the result of the sterical hindrance and hence repulsion between the first aromatic ring of the 4-phenanthrenyl radical and the vinylacetylene molecule adding with the methylidene moiety (CH_2) to the aryl radical center. In our present study, the sterical hindrance for the reactions of the [4] and [5]helicenyl radicals with vinylacetylene is significantly reduced due to the positioning of the attacked radical site outside of the molecular "bay" thus lowering the barrier heights below the energy of the separated reactants hence resulting in a submerged barrier. In this sense, the features in the entrance channels of the reactions to [5] and [6]helicene are quite distinct from those of the reaction of the 4-phenanthrenyl radical ($C_{14}H_9$) with vinylacetylene (C_4H_4) leading to [4]helicene.[28] To explore the implications of our findings to the chemistry of aromatic hydrocarbons in cold molecular clouds, we explored the viability of the formation of polycyclic aromatic hydrocarbons via neutral-neutral reactions exploiting the University of Manchester Institute for Science and Technology (UMIST) Database (RATE2012).[43] The models were operated with physical parameters updated from References [43] and [46]: a cosmic ray ionization rate of 1.3×10^{-17} s^{-1}, a temperature of 10 K, a visual extinction of 10 Mag, and a number density of molecular hydrogen of 10^4 cm^{-3}. This network was updated with recently explored barrierless and rapid reactions related to the formation of benzene (C_6H_6),[44] naphthalene ($C_{10}H_8$),[45] phenanthrene ($C_{14}H_{10}$),[47] and [4]helicene[48] along with the channels to [5]helicene and [6]helicene elucidated in the present work (Figure 6, Table S2). Reaction pathways to benzene (C_6H_6) were extracted from Reference [44] (Materials and Methods; †ESI).

These modeling studies reveal fascinating conclusions. *First*, the performance of the astrochemical model for the cold molecular cloud TMC-1 can be benchmarked for the cyano derivatives of benzene (C_6H_6) and naphthalene ($C_{10}H_8$), i.e. cyanobenzene (C_6H_5CN), and 1- and 2-cyanonapthalene ($C_{10}H_8CN$), which were recently observed at fractional abundances of $4 \pm 1.6 \times 10^{-11}$ [49] as well as $7.35\,^{+3.33}_{-4.63} \times 10^{-11}$ and $7.05\,^{+3.23}_{-4.50} \times$

10^{-11} toward TMC-1.[50] Formed predominantly via the barrierless reactions of benzene and naphthalene with cyano radicals,[51,52] the predicted peak fractional abundances at 2×10^5 years of cyanobenzene (C_6H_5CN) and both cyanonapthalene ($C_{10}H_8CN$) isomers with respect to molecular hydrogen reproduce the astronomical observations exceptionally well (Figure 7). *Second*, barrierless molecular mass growth processes via ring annulation lead from two-ring PAHs ($C_{10}H_8$; naphthalene) via three ($C_{14}H_{10}$; phenanthrene), four ($C_{18}H_{12}$; [4]helicene), five ($C_{22}H_{14}$; [5]helicene), and six-ring PAHs ($C_{26}H_{16}$; [6]helicene). With increasing complexity, the fractional abundances decrease from a few 10^{-8} for naphthalene via 2×10^{-9} for phenanthrene and 3×10^{-10} for [4]helicene to nearly 10^{-11} for [5]helicene and 8×10^{-14} for [6]helicene. This implies that in future observations, at least three to five ringed PAHs including [4] and [5]helicenes might be detectable by radio telescopes.

Conclusion

Our combined experimental, computational, and astrochemical modeling results provided compelling evidence on a versatile, barrierless molecular mass growth process to helicenes via ring annulation in cold molecular clouds (10 K) as the result of bimolecular reactions of helicenyl radicals with vinylacetylene in the gas-phase. Commencing with the photolysis of an [*n*]helicene [$C_{14+4n}H_{10+2n}$] to an [n]helicenyl radical [$C_{14+4n}H_{9+2n}$] through the internal ultraviolet field (reaction (3)),[53] this universal mechanism effectively converts an [*n*]helicene into an [*n*+1]helicene [$C_{14+4(n+1)}H_{10+2(n+1)}$] (reaction (4)).

(3) $$C_{14+4n}H_{10+2n} + h\upsilon \rightarrow C_{14+4n}H_{9+2n} + H$$

(4) $$C_{14+4n}H_{9+2n} + C_4H_4 \rightarrow C_{14+4(n+1)}H_{10+2(n+1)} + H$$

The gas-phase synthesis of helicenes may have profound implications for the origin of the chiral asymmetry of life and contemporary biorelevant molecules such as right-handed sugars and left- handed amino acids. Although the gas-phase processes unraveled here form *racemates* of [5] and [6]helicenes, in deep space, ultraviolet circularly polarized light may preferentially photolyze the **M** or **P** enantiomer; this process could lead to an enrichment

of one enantiomer over the other (enantiomeric excess), which can be propagated by the further growth. Since PAHs, to which helicene belongs, represent fundamental molecular building blocks of nanometer-sized interstellar grains,[54-59] a bottom-up formation of carbonaceous nanoparticles via PAHs leads to chiral carbonaceous nanostructures[26,27,55,56,60] and may translate the enantiomeric excess of the helicenes from the gas-phase to the nanoparticles eventually resulting into *chiral islands* or *chiral surfaces*. Although there is no detailed description to date of how carbonaceous nanoparticles might form in deep space, PAHs are likely key contributors. Consequently, the work disseminated here signifies a critical advancement toward a systematic understanding of the fundamental chemical processes forming carbonaceous grains in the interstellar medium. At low temperatures of cold molecular clouds (10 K), these grains accrete nanometer thick icy layers of, e.g., water, carbon monoxide, carbon dioxide, formaldehyde, methanol, methane, and ammonia.[61] Interaction of interstellar ices with ionizing radiation such as galactic cosmic rays and the internal ultraviolet field[62] revealed the synthesis of complex organic molecules of astrobiological significance such as amino acids,[11-15] dipeptides,[63] and even sugars at 10 K.[16] In the presence of *chiral islands* and *chiral surfaces*, a grain-surface-mediated synthesis may lead to an enantiomeric excess within the newly formed molecules like sugars and amino acids. Therefore, these biorelevant molecules, which have been enantiomerically enriched through a chiral surface-mediated low temperature ice-surface chemistry in molecular clouds, could have been eventually delivered to the early Earth. This scenario gains strong support from the recent identification of D-enriched sugar alcohols and sugar acids like arabinonic acid[7] along with L-enriched non-terrestrial amino acids such as isovaline, α-methyl norvaline, α-methyl valine, and α-methyl norleucine in Murchison and Murray carbonaceous meteorites[8] thus bringing us closer to the understanding of the origin of homochirality.

Data Availability

The datasets generated during this study are available upon request.

Acknowledgements

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Author Contributions

R.I.K. designed the experimental program and guided the astrochemical models; W.L. and L.Z. performed the experiments under the supervision of M.A.; M.M.E., V.N.A., and A.M.M. conducted the electronic structure and RRKM calculations; R.K.M. synthesized the precursors under supervision by F.R.F.; R.I.K. and M.A. wrote the manuscript. X.L. conducted the astrochemical modeling.

Competing Interests

The authors declare no competing interests.

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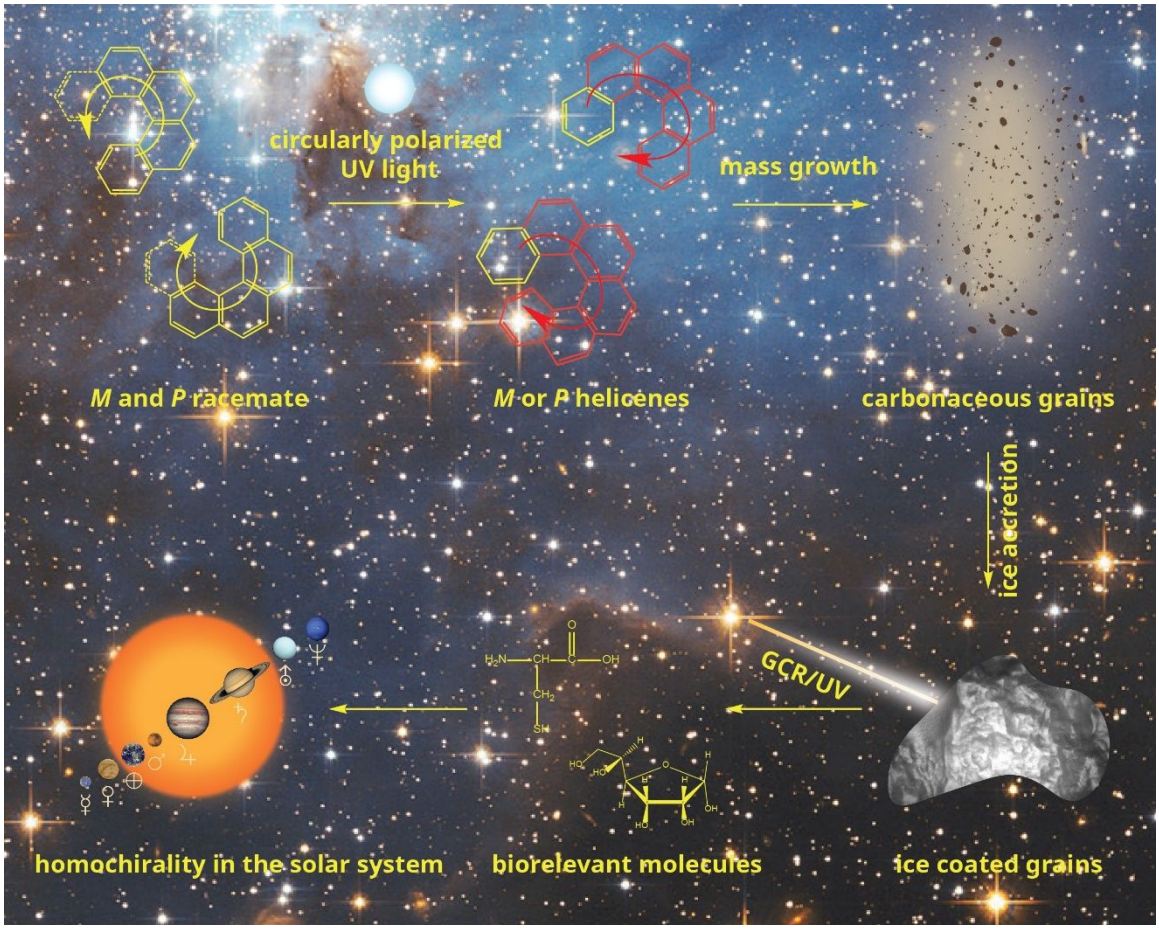

Fig. 1. Overview of the role of racemic helicenes in the enantiomeric of sugars and amino acids in meteorites. Racemic mixtures of [5] and [6]helicenes can form in the gas-phase of the interstellar medium at ultralow temperatures in the absence of reaction barriers via molecular mass growth processes. Ultraviolet circularly polarized light may then preferentially photolyze one of the enantiomers leading to an enrichment of one enantiomer over the other. Polycyclic aromatic hydrocarbons (PAHs) – including enantiomerically enriched helicenes - can be incorporated into carbonaceous grains through molecular mass growth resulting into chiral islands or chiral surfaces. Upon interaction with galactic cosmic rays and ultraviolet photons, enantiomerically enriched complex organic molecules of astrobiological significance like sugars and aminoacids may be synthesized on ice coated chiral grains. Enantiomerically enriched biorelevant molecules could have been eventually delivered to early Earth. This brings us closer to the understanding of the origin of homochirality.

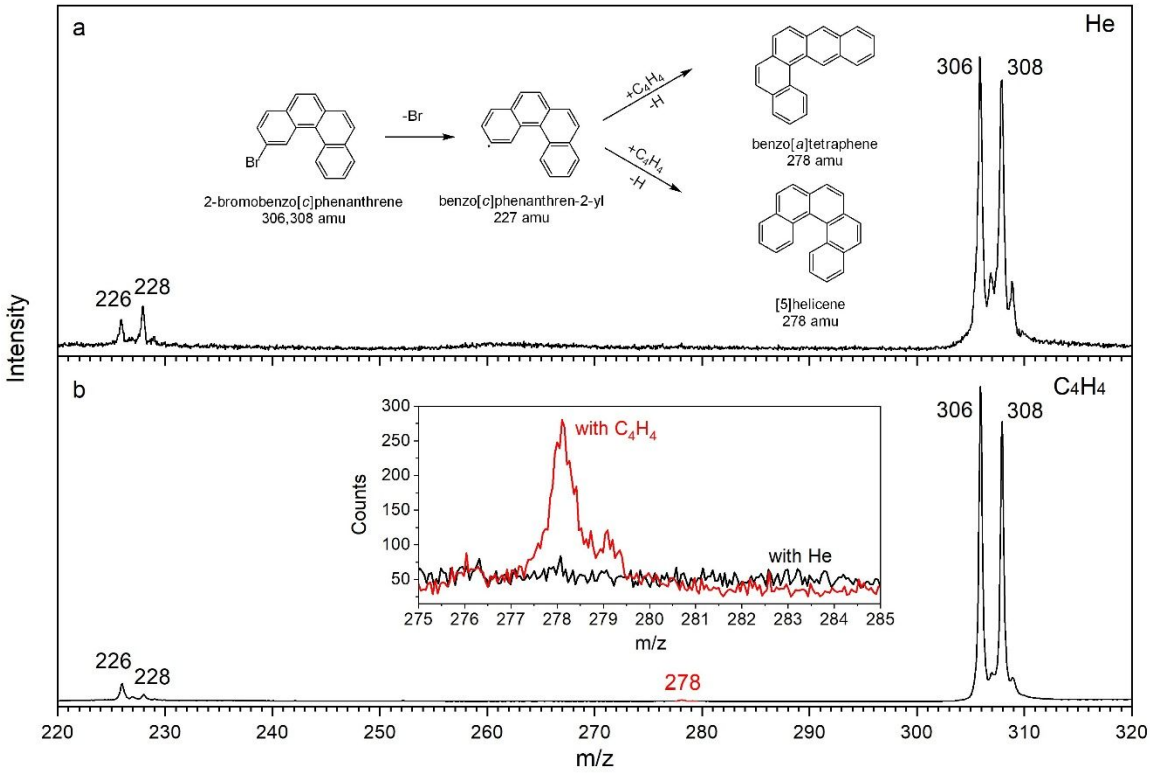

Fig. 2. Comparison of photoionization mass spectra recorded at a photon energy of 9.50 eV. (a) 2-bromobenzo[*c*]phenanthrene ($C_{18}H_{11}Br$) - helium (He) system; (b) 2-bromobenzo[*c*] phenanthrene ($C_{18}H_{11}Br$) - vinylacetylene (C_4H_4) system. The inset of (a) represents the formation of benzo[*a*]tetraphene ($C_{22}H_{14}$) and [5]helicene ($C_{22}H_{14}$) from the reaction of the benzo[*c*]phenanthren-2-yl radical ($C_{18}H_{11}^{\bullet}$) with vinylacetylene (C_4H_4). The benzo[*c*]phenanthren-2-yl radical is produced from the pyrolysis of 2-bromobenzo[*c*]phenanthrene ($C_{18}H_{11}Br$). The inset of (b) shows the mass peak of the newly formed species of interest along with the ^{13}C-counterparts in red.

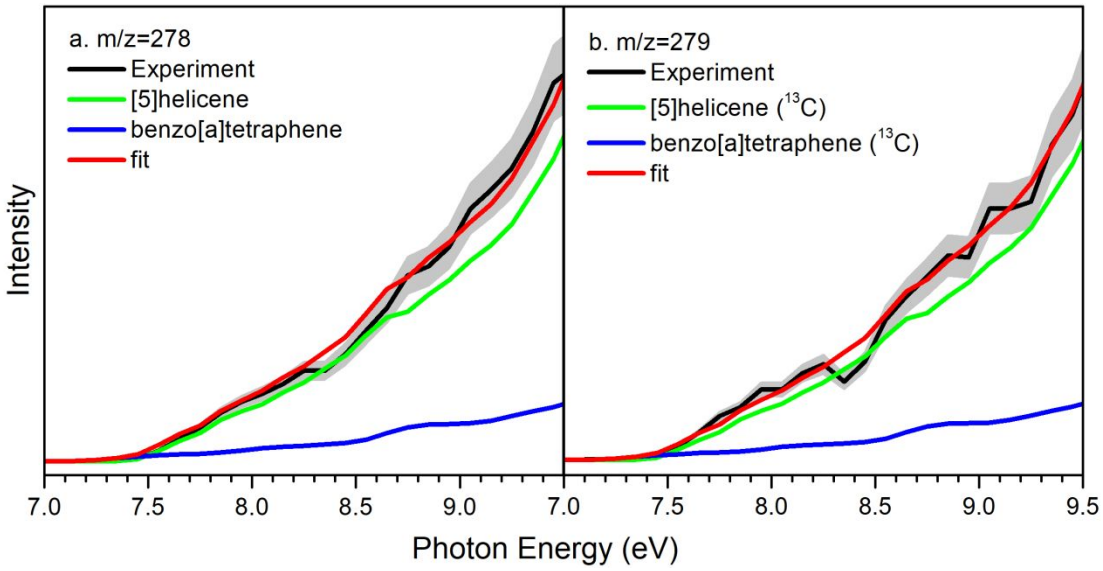

Fig. 3. Photoionization efficiency (PIE) curves of *m*/*z* = 278 and 279 for the reaction of 2-bromobenzo[*c*]phenanthrene ($C_{18}H_{11}Br$) - vinylacetylene (C_4H_4). Black: experimentally derived PIE curves; colored lines (green and blue): reference PIE curves; red lines: overall fit. The overall error bars consist of two parts: ± 10 % based on the accuracy of the photodiode and a 1 σ error of the PIE curve averaged over the individual scans.

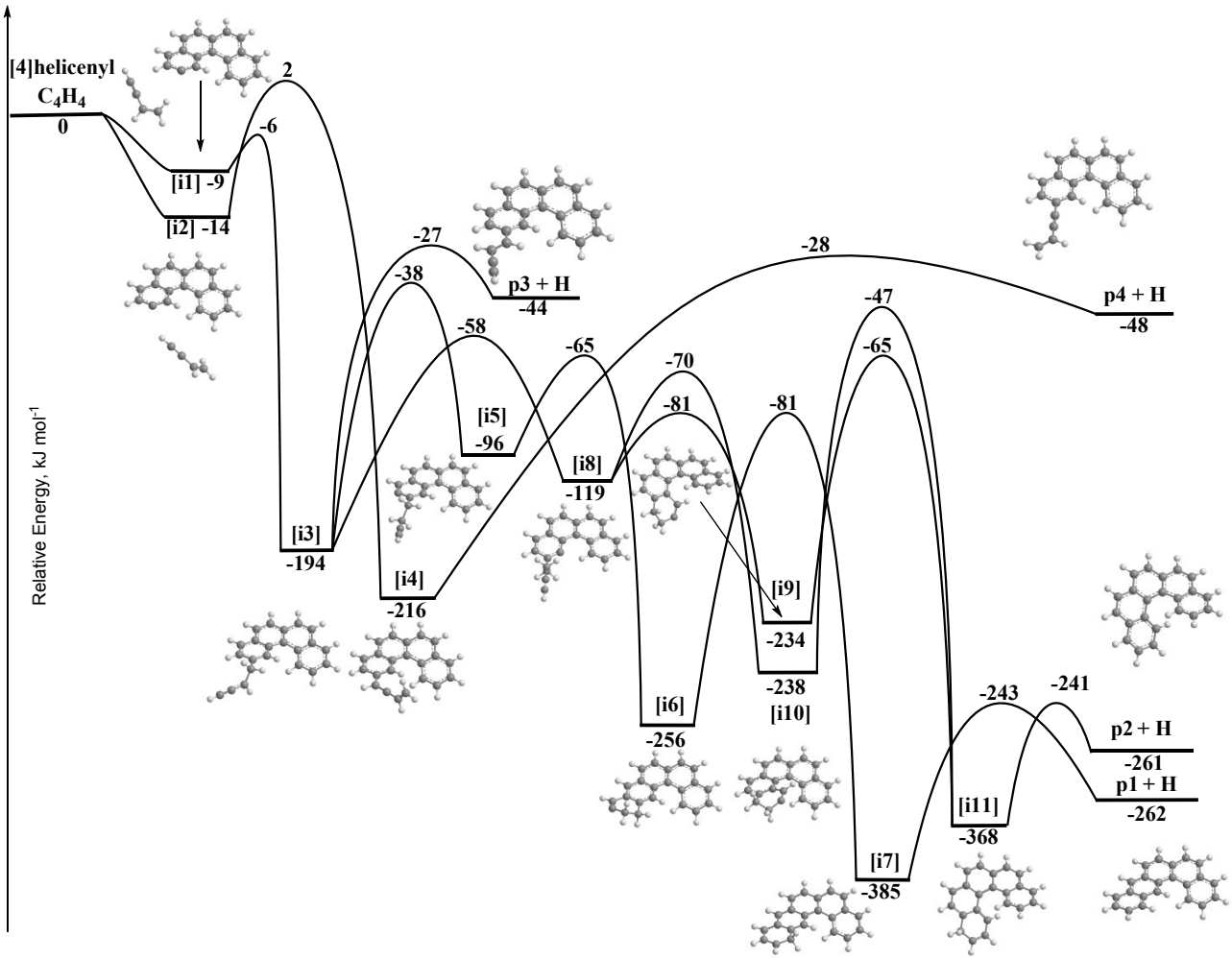

Fig. 4. Potential energy surface (PES) for the [4]helicenyl ($C_{18}H_{11}$•) reaction with vinylacetylene (C_4H_4) leading to [5]helicene ($C_{22}H_{14}$). This PES was calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory. The relative energies are given in kJ mol^{-1}.

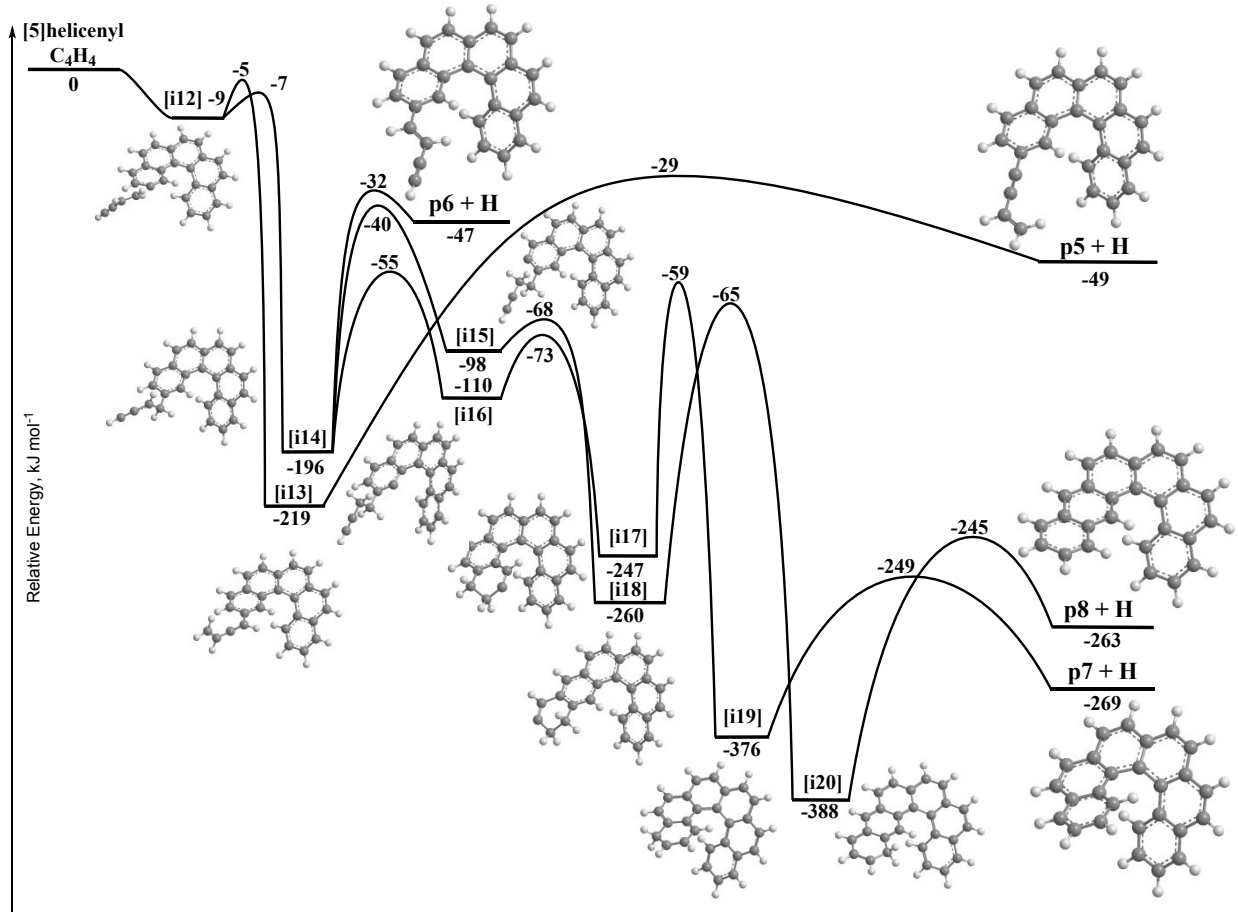

Fig. 5. Potential energy surface (PES) for the [5]helicenyl ($C_{22}H_{13}$•) reaction with vinylacetylene (C_4H_4) leading to [6]helicene ($C_{26}H_{16}$). This PES was calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory. The relative energies are given in kJ mol^{-1}.

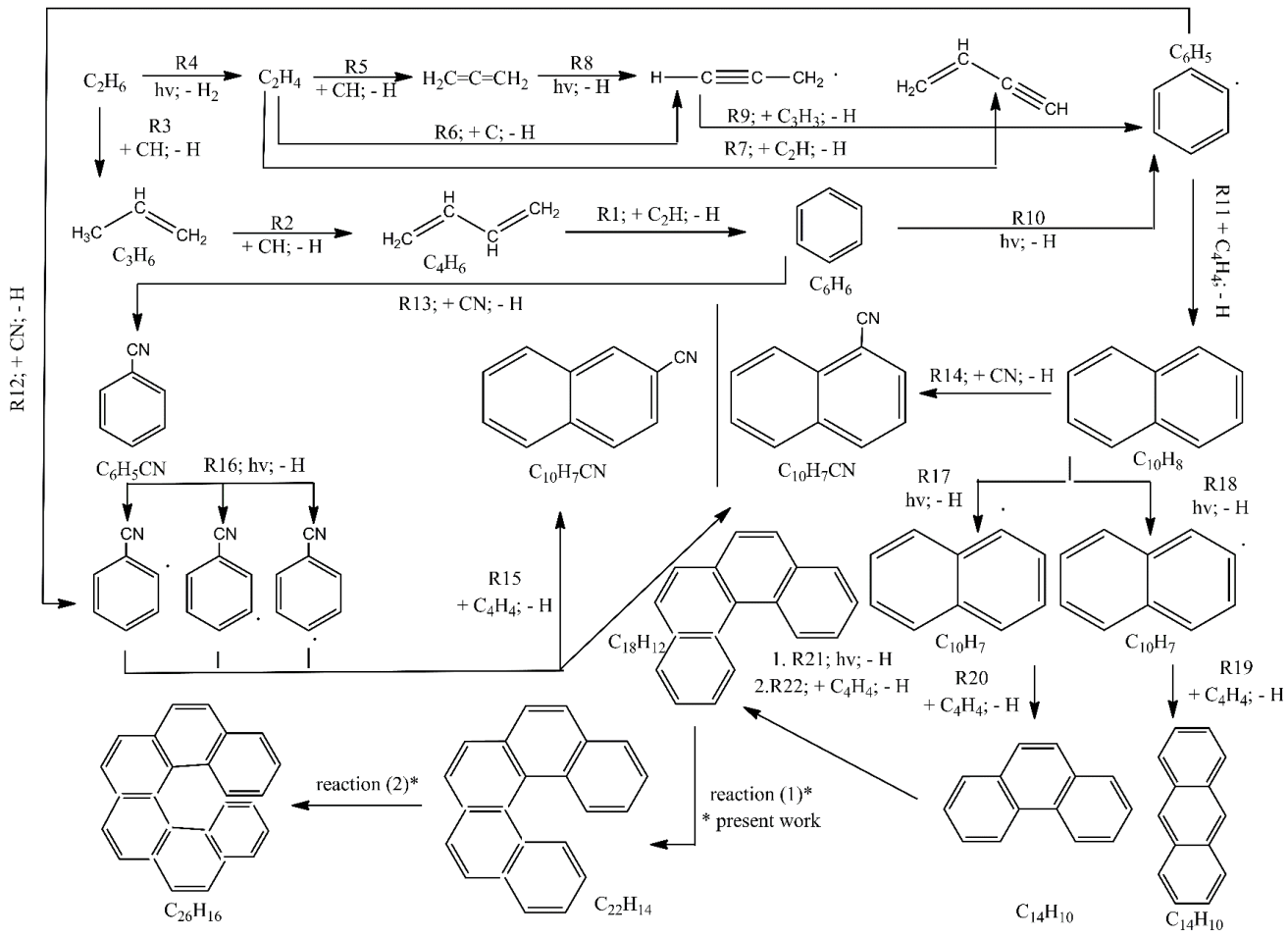

Fig. 6. Compilation of key bimolecular reactions leading to aromatic molecules as incorporated into the novel astrochemical models. The reactions R1-R22 are discussed in the Supplementary Information.

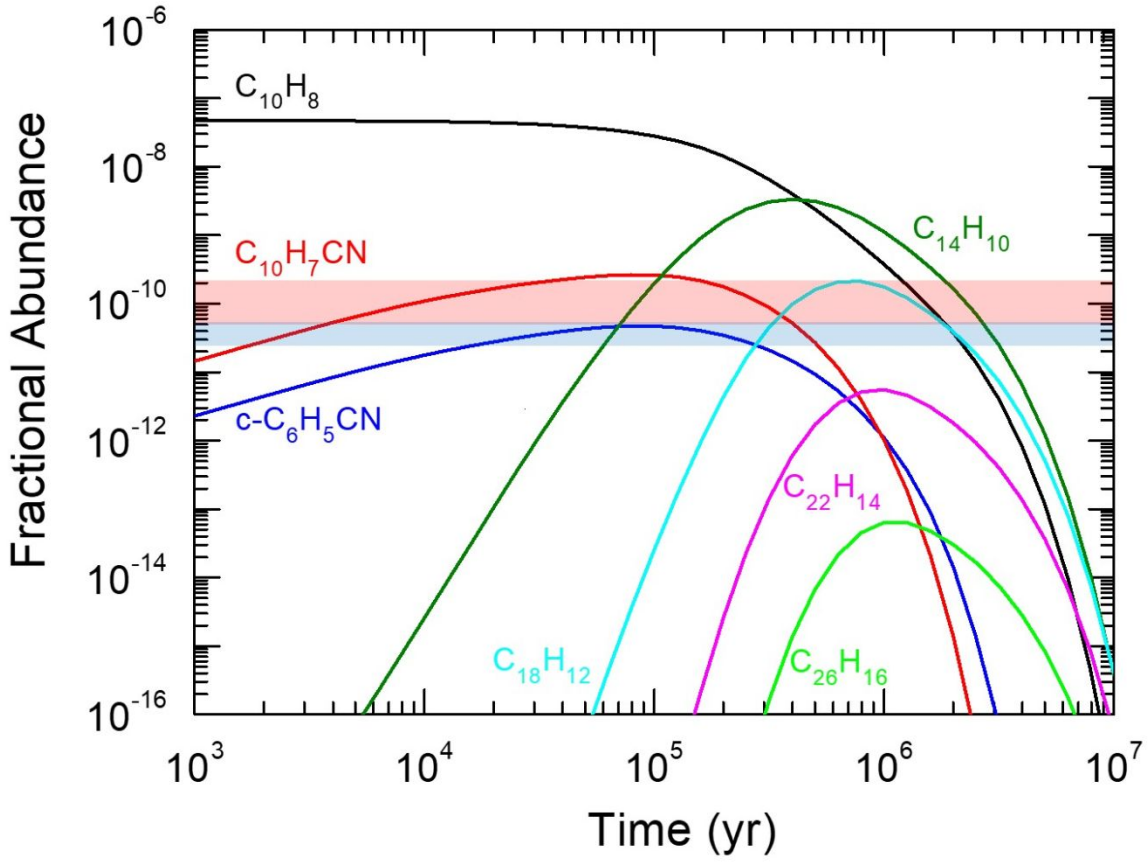

Fig. 7. Results of the astrochemical modeling for key pathways leading eventually to the formation of helicenes in TMC-1. The fractional abundances of the gas-phase species (($C_{10}H_8$; naphthalene), ($C_{14}H_{10}$; phenanthrene), ($C_{18}H_{12}$; [4]helicene), ($C_{22}H_{14}$; [5]helicene), and ($C_{26}H_{16}$; [6]helicene)) are plotted versus time for the cold molecular cloud TMC-1. Astronomically observed fractional abundances along with the uncertainties of cyanobenzene (C_6H_5CN) and cyanonapthalenes ($C_{10}H_7CN$) are visualized by the blue and red color-coded bars and agree nicely with the peak abundances predicted from the present models.

Supplementary Materials for

Gas-Phase Synthesis of Racemic Helicenes and their Potential Role in the Enantiomeric Enrichment of Sugars and Amino Acids in Meteorites

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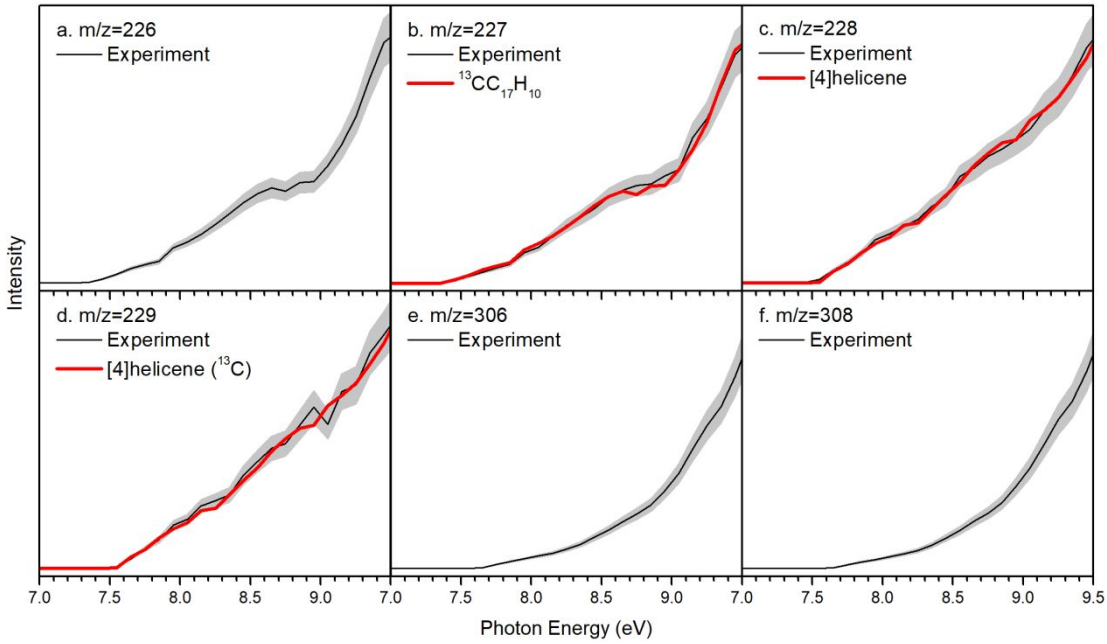
Fig. S1.



Photoionization efficiency (PIE) curves for reaction of 2-bromobenzo[*c*]phenanthrene - bromo[4]-helicene ($C_{18}H_{11}Br$) - vinylacetylene (C_4H_4). Black: experimentally derived PIE curves; red lines: reference PIE curves. The overall error bars consist of two parts: ±10% based on the accuracy of the photodiode and a 1 σ error of the PIE curve averaged over the individual scans. The PIE curves for m/z = 308 and 306 are superimposable and can be connected to 2-bromobenzo[*c*]phenanthrene: $C_{18}H_{11}{}^{79}Br^+$ (*m/z* = 306) and $C_{18}H_{11}{}^{71}Br^+$ (*m/z* = 308). Likewise, the PIE graphs for m/z = 229 and 228 essentially overlap. Both PIE curves can be replicated through a reference PIE for [4]helicene ($C_{18}H_{12}$; *m/z* = 228) and ^{13}C-[4]helicene ($^{13}CC_{17}H_{12}$; *m/z* = 229). Finally, the PIE curves at m/z = 226 and 227 also overlap.

Table S1.

Optimized Cartesian coordinates and calculated vibrational frequencies of various structures involved in the [4]/[5]helicenyl plus vinylacetylene reactions.

Structure	Cartesian Coordinates, Å			Frequencies, cm^{-1}		
[i1]	C	-2.385414	0.686641	0.006817		
	C	-3.803768	0.634145	0.190151	5.7183	9.9521	11.2011
	C	-1.821292	1.964876	-0.241862	25.3016	33.7357	46.3059
	C	-1.629229	-0.556218	-0.015088	80.4067	84.5265	129.8663
	C	-4.550515	1.832656	0.269927	178.4983	211.5812	228.0577
	C	-4.468573	-0.627954	0.215116	260.6443	279.0589	319.2188
	C	-2.578295	3.116835	-0.193385	325.2711	378.1449	411.3631
	C	-2.353445	-1.766223	-0.142970	438.3684	441.1753	477.4842
	C	-3.951319	3.059498	0.102053	511.3366	525.6124	526.7687
	C	-3.775619	-1.774603	-0.008000	552.6375	559.6069	575.1462
	C	-0.182830	-0.646285	0.087736	592.9689	623.2409	645.1824
	C	-1.673016	-2.993347	-0.407261	672.0826	680.9936	686.3094
	C	0.468167	-1.884486	-0.224699	703.4770	703.8604	749.2939
	C	-0.319119	-3.040246	-0.508006	757.5318	759.7134	780.4124
	C	1.880072	-1.989748	-0.179721	805.0030	824.7806	828.4965
	C	2.674663	-0.932326	0.223973	851.1921	855.8644	876.4762
	C	0.648279	0.403437	0.588882	892.3387	895.4254	958.0447
	C	1.992113	0.210307	0.612933	958.2770	964.6310	967.1520
	C	5.270168	2.209989	-0.803122	975.3878	982.7567	1001.5523
	C	6.411837	1.542090	-0.607524	1009.5098	1012.7253	1057.2972
	C	6.563377	0.448140	0.289942	1078.3746	1112.5044	1123.5548
	C	6.733127	-0.480131	1.039370	1147.1293	1171.2662	1175.3405
	H	-0.784964	2.044144	-0.532471	1183.8721	1205.1928	1223.5573
	H	-5.620208	1.762980	0.437913	1235.4304	1246.1712	1263.7554
	H	-5.543604	-0.647628	0.358594	1307.8527	1322.1524	1343.0992
	H	-2.110436	4.071879	-0.404455	1351.1593	1369.2208	1394.4673
	H	-4.537000	3.969972	0.156607	1410.5434	1440.0933	1446.2112
	H	-4.289663	-2.728179	-0.064307	1451.8173	1471.9905	1498.9977
	H	-2.267926	-3.889236	-0.548717	1530.3881	1545.4483	1588.3683
	H	0.187224	-3.968724	-0.748766	1611.4552	1635.7873	1647.8337
	H	2.336811	-2.936579	-0.451449	1665.3080	1668.2635	2202.1090
	H	3.755303	-1.007772	0.257056	3135.1571	3144.2610	3153.6236
	H	0.211164	1.303394	0.996498	3157.3575	3159.4729	3161.0450
	H	5.225934	3.034435	-1.504446	3169.8949	3176.7392	3179.2112
	H	4.359059	1.951279	-0.276346	3181.4241	3186.2930	3201.7969
	H	7.305148	1.829699	-1.156602	3227.3863	3233.8016	3476.1453
	H	6.876944	-1.291954	1.709324			
[i2]	C	0.430177	-1.335679	0.197596	7.5397	12.8417	20.9298
	C	0.786312	-2.721109	0.243104	26.3244	31.1046	51.2538
	C	-0.954605	-1.030043	0.248157	80.6381	85.3721	129.3097
	C	1.478047	-0.344210	0.006872	178.6144	211.8463	226.9192
	C	-0.207345	-3.698049	0.484982	260.6936	278.6879	320.1681
	C	2.129238	-3.117097	-0.031338	325.1794	378.0490	411.5998
	C	-1.908157	-2.006038	0.451055	438.3079	441.0495	477.8265
	C	2.751832	-0.801095	-0.410065	510.5000	525.4634	526.9800
	C	-1.532981	-3.351501	0.608736	552.2654	557.6400	574.4150
	C	3.055454	-2.197002	-0.405982	593.5149	623.0263	671.5965
	C	1.314206	1.083509	0.219308	679.7437	686.7151	703.0625
	C	3.749646	0.125881	-0.838805	703.9643	706.0716	747.6788
	C	2.318947	1.986495	-0.260030	758.0892	759.4220	777.1093
	C	3.520764	1.464823	-0.825009	806.6078	824.5121	826.7659
	C	2.163523	3.386335	-0.109271	851.2242	855.2223	878.4794
	C	1.078175	3.927821	0.554727	892.2184	898.7005	952.2733
	C	0.250103	1.658124	0.981776	954.1869	958.0607	967.1468
	C	0.184984	3.010477	1.087450	975.9231	983.3366	1007.3490
	C	-3.469633	2.249419	0.029648	1010.4228	1013.8794	1056.9460
	C	-4.440972	1.564596	-0.170160	1078.3606	1111.6480	1122.1765
	C	-5.608835	0.777584	-0.372151	1145.4276	1171.6603	1174.6695
	C	-5.722464	-0.189091	-1.289562	1184.3819	1205.1686	1223.2123
	H	-1.292705	-0.021155	0.068442	1235.6295	1245.5450	1263.8811
	H	0.095913	-4.738317	0.542068	1307.5352	1320.9958	1342.6090
	H	2.379847	-4.171704	0.010399	1351.0637	1369.0777	1394.3159
	H	-2.955617	-1.727570	0.470042	1409.9720	1439.3551	1443.6122

	H	-2.285583	-4.111307	0.786041	1451.6742	1471.6733	1498.2693
	H	4.057025	-2.504303	-0.687227	1530.2160	1545.3158	1588.2002
	H	4.693932	-0.268024	-1.198988	1610.7886	1635.4715	1647.3479
	H	4.269539	2.159547	-1.189739	1665.1277	1666.3604	2200.8038
	H	2.933043	4.038510	-0.510869	3134.7248	3146.3025	3154.1710
	H	0.958158	4.998657	0.669061	3157.1686	3159.3581	3161.1382
	H	-0.452044	1.027440	1.507434	3172.7092	3176.7718	3179.3026
	H	-2.601110	2.840665	0.197228	3181.8053	3186.8767	3203.4352
	H	-6.450597	1.001778	0.278696	3230.2254	3235.5035	3454.8819
	H	-4.905579	-0.437963	-1.956490			
	H	-6.642710	-0.751154	-1.392314			
	C	-1.584885	-0.368310	0.189299			
	C	-2.961122	-0.305922	-0.187919	65.0183	71.7766	90.1923
	C	-1.165325	-1.512612	0.912787	121.1340	169.4430	174.6380
	C	-0.722475	0.782154	-0.054874	229.2821	245.9173	275.9626
	C	-3.800847	-1.424617	0.027396	312.8460	343.1501	399.0500
	C	-3.502038	0.916243	-0.691185	420.0448	420.9253	451.1723
	C	-2.014086	-2.572040	1.149200	471.3168	477.4819	496.2063
	C	-1.365261	2.017949	-0.331427	527.0924	537.3847	545.3051
	C	-3.337820	-2.547753	0.672475	552.1590	576.6696	611.3338
	C	-2.748081	2.045648	-0.694572	635.1522	659.9005	679.1740
	C	0.722491	0.782080	0.055069	691.7067	724.6865	736.0635
	C	-0.648187	3.240027	-0.208658	753.5254	765.7199	779.0054
	C	1.365397	2.017841	0.331468	785.5749	798.3978	805.1901
	C	0.648433	3.239972	0.208599	817.2553	840.1081	856.5633
	C	2.748241	2.045490	0.694526	866.7740	884.2181	884.9030
	C	3.502166	0.916066	0.691112	937.6227	949.7448	960.8174
	C	1.584861	-0.368436	-0.189183	967.4285	969.4292	978.1861
p2	C	2.961131	-0.306073	0.187869	981.4815	997.5197	998.7557
	C	1.165107	-1.512755	-0.912514	1047.2512	1058.7675	1082.8936
	C	2.013832	-2.572199	-1.149041	1094.7569	1151.2859	1166.2608
	C	3.337674	-2.547866	-0.672696	1171.9946	1179.5497	1183.4292
	C	3.800806	-1.424741	-0.027639	1184.6747	1207.9627	1225.0696
	H	-0.159857	-1.550366	1.305784	1234.3876	1239.0666	1249.2464
	H	-4.834694	-1.364027	-0.296461	1286.0935	1297.8467	1343.8618
	H	-4.543626	0.941837	-0.993011	1357.0025	1364.7573	1374.2517
	H	-1.659145	-3.424962	1.716611	1398.0421	1412.0161	1448.1889
	H	-3.995068	-3.392516	0.844626	1448.7082	1466.1003	1472.5462
	H	-3.182088	2.998918	-0.977139	1515.1134	1526.5749	1547.0843
	H	-1.172426	4.171147	-0.394752	1555.0192	1590.2931	1623.0281
	H	1.172769	4.171059	0.394592	1647.5104	1649.1120	1655.7888
	H	3.182296	2.998752	0.977062	1661.4907	3157.4521	3157.8519
	H	4.543764	0.941639	0.992884	3159.6895	3160.2138	3162.1974
	H	0.159534	-1.550531	-1.305244	3170.8120	3170.9482	3176.9954
	H	1.658755	-3.425233	-1.716206	3177.8707	3180.7635	3186.2770
	H	3.994964	-3.392528	-0.845178	3186.5756	3217.8432	3218.5106
	H	4.834757	-1.364078	0.295886			
	C	-2.045629	-0.506256	0.093042	57.0800	63.5956	90.6676
	C	-3.429126	-0.307476	-0.222742	122.5918	154.5401	196.5787
	C	-1.679372	-1.793305	0.570820	218.0040	255.3773	289.3989
	C	-1.133592	0.619141	0.006482	309.4124	321.8994	399.9702
	C	-4.324290	-1.403875	-0.197280	404.0620	415.6479	438.8257
	C	-3.910538	1.005298	-0.491084	473.6963	483.7897	503.7550
	C	-2.580686	-2.834385	0.621322	523.5619	531.5439	538.6028
	C	-1.691292	1.910794	-0.106925	572.1504	589.4655	601.3448
	C	-3.910544	-2.653480	0.198229	636.8863	651.1020	663.9033
	C	-3.081594	2.077757	-0.373480	713.7306	717.9230	747.3337
	C	0.325432	0.509608	0.028727	756.3666	763.0430	775.7166
p1	C	-0.869881	3.077267	0.060062	790.2634	806.5512	810.2426
	C	1.111821	1.702154	0.256635	818.0069	842.2834	846.8700
	C	0.458206	2.977194	0.301421	859.9764	883.3713	902.6825
	C	2.499971	1.620540	0.340908	916.9969	926.6146	949.7424
	C	3.188879	0.417830	0.139346	964.8218	968.2832	977.7305
	C	1.024629	-0.665156	-0.257018	982.5310	995.0028	1003.7684
	C	2.426363	-0.747126	-0.208517	1023.7308	1032.7939	1066.5931
	C	4.608734	0.316401	0.211226	1110.9464	1157.5953	1162.5774
	C	5.240073	-0.868143	-0.057523	1172.6617	1181.5282	1184.4721
	C	4.487578	-2.018714	-0.419321	1195.7494	1214.9688	1229.5257
	C	3.121972	-1.958144	-0.495657	1236.1369	1257.3734	1285.8937
	H	-0.685305	-1.953565	0.959480	1292.3920	1313.3222	1355.1715

	H	-5.359854	-1.229195	-0.470121	1356.2081	1375.4826	1383.2547
	H	-4.959072	1.137679	-0.735392	1401.8485	1418.7510	1445.9489
	H	-2.264370	-3.795906	1.010085	1449.5014	1454.7880	1480.3869
	H	-4.608826	-3.482230	0.223032	1509.3505	1523.3177	1542.1899
	H	-3.462390	3.085315	-0.502605	1577.7889	1592.5582	1630.2171
	H	-1.351957	4.048305	0.020898	1631.6180	1648.5258	1666.1383
	H	1.061045	3.862330	0.473538	1669.9438	3155.5381	3157.5487
	H	3.065799	2.528288	0.527369	3158.0321	3159.6895	3161.3174
	H	0.488877	-1.548168	-0.573226	3162.4522	3169.8863	3175.4777
	H	5.181597	1.198286	0.478488	3177.3386	3179.6283	3186.7293
	H	6.320702	-0.934618	-0.000123	3188.0587	3206.8841	3227.7721
	H	5.004162	-2.947341	-0.634262			
	H	2.546905	-2.836726	-0.769197			
p3	C	1.883055	0.823439	0.114438			
	C	3.226195	1.119416	-0.281569	34.2210	58.9351	72.9700
	C	1.137082	1.886889	0.686304	87.6128	95.1859	123.6356
	C	1.400255	-0.544167	0.007605	159.8853	182.5966	223.0483
	C	3.697605	2.452121	-0.237598	239.8714	271.6815	280.7827
	C	4.107829	0.058193	-0.645376	321.7176	368.6573	387.8235
	C	1.633337	3.171998	0.750547	418.4649	433.1447	443.7842
	C	2.357893	-1.565879	-0.202427	465.7746	482.8817	502.7307
	C	2.912633	3.471025	0.250361	533.3691	537.0881	548.5204
	C	3.705001	-1.234928	-0.544790	584.9433	594.7804	618.3368
	C	0.003635	-0.940594	0.099897	625.1897	639.1427	680.5553
	C	1.990573	-2.939242	-0.074761	690.9512	702.1133	709.3740
	C	-0.316537	-2.323229	0.273868	757.2983	759.3506	767.3005
	C	0.713174	-3.303736	0.218146	799.1317	810.0333	823.5906
	C	-1.671209	-2.710718	0.425359	835.9799	837.0513	858.0817
	C	-2.694073	-1.804870	0.331000	864.2081	885.5454	907.8414
	C	-1.084102	-0.052268	-0.075544	930.3049	962.7725	967.8969
	C	-2.413880	-0.446375	0.031856	976.2796	982.7919	986.9824
	C	-3.455881	0.552691	-0.188291	991.0396	1005.3082	1024.1963
	C	-4.789705	0.365504	-0.114315	1046.7609	1067.9368	1127.2259
	C	-5.740403	1.391203	-0.338170	1160.2924	1173.3196	1183.2360
	C	-6.576681	2.240514	-0.522448	1185.4423	1207.0348	1228.7785
	H	0.177351	1.683893	1.136646	1237.2671	1244.9503	1260.1477
	H	4.710666	2.651696	-0.570956	1283.2203	1298.6134	1327.4182
	H	5.120781	0.302667	-0.946617	1338.1562	1353.6331	1371.9774
	H	1.036644	3.952221	1.209549	1388.2759	1398.3051	1427.4274
	H	3.289891	4.486518	0.287444	1450.9155	1460.3767	1478.9067
	H	4.396373	-2.046019	-0.746761	1523.9276	1539.5608	1555.4915
	H	2.764321	-3.689946	-0.194681	1588.5438	1631.8444	1647.5118
	H	0.450331	-4.347083	0.355234	1648.8585	1660.0829	1665.8374
	H	-1.889559	-3.760124	0.593726	2193.9386	3143.1189	3153.1082
	H	-3.717526	-2.140025	0.446051	3157.6751	3159.4312	3160.8849
	H	-0.888950	0.970854	-0.360843	3162.9383	3170.4807	3177.0890
	H	-3.101657	1.549742	-0.435002	3179.4186	3186.6518	3189.2934
	H	-5.197746	-0.611447	0.128783	3208.0229	3227.5907	3477.3975
	H	-7.305703	2.995123	-0.687109			
p4	C	1.836855	0.866758	0.122146	32.7038	41.6295	50.4328
	C	3.156599	1.249183	-0.279276	81.2916	94.9054	117.3656
	C	1.029288	1.877641	0.705963	163.0249	165.6755	202.3204
	C	1.440212	-0.527430	0.006746	254.2740	270.0613	288.7863
	C	3.544537	2.608356	-0.227129	319.7626	336.6531	379.4466
	C	4.100091	0.248458	-0.657829	411.5020	427.3791	446.8301
	C	1.445208	3.190427	0.777553	470.3864	479.8347	500.5515
	C	2.457777	-1.485007	-0.218915	530.3527	538.7429	549.9852
	C	2.700660	3.572473	0.273253	584.8964	589.6175	627.6339
	C	3.779095	-1.068196	-0.566765	636.3897	656.7103	692.0329
	C	0.070690	-1.011649	0.106003	694.2149	707.2942	710.3998
	C	2.178261	-2.880454	-0.099929	757.8468	766.0782	782.6100
	C	-0.161252	-2.414667	0.271743	802.7445	810.2055	831.0021
	C	0.929701	-3.327120	0.199761	840.3536	862.1535	874.0158
	C	-1.484354	-2.892673	0.429383	885.0827	932.6774	939.1181
	C	-2.565346	-2.053465	0.351408	951.7603	965.2207	971.0492
	C	-1.067178	-0.188261	-0.054234	978.3793	983.6489	993.6796
	C	-2.365514	-0.677865	0.064696	1006.5149	1006.6973	1036.0997
	C	-3.480481	0.184869	-0.118580	1067.5212	1102.2686	1129.3007
	C	-4.443838	0.904240	-0.268748	1159.9314	1173.1063	1179.9330
	C	-5.539549	1.782827	-0.455221	1184.9402	1210.0284	1230.8885

	C	-6.829031	1.434772	-0.348660	1237.8130	1250.4063	1273.5334
	H	0.085639	1.613350	1.158268	1291.6090	1319.3802	1326.9018
	H	4.541167	2.873060	-0.564672	1346.3404	1365.1755	1385.7829
	H	5.093812	0.558191	-0.963113	1396.1492	1420.3153	1445.6220
	H	0.803126	3.928438	1.244993	1451.4311	1462.6736	1476.1608
	H	3.014098	4.609231	0.316386	1518.5337	1538.7670	1550.4424
	H	4.518147	-1.832932	-0.780420	1585.9514	1630.0180	1644.5238
	H	2.997027	-3.579729	-0.231439	1647.7591	1663.7513	1665.9243
	H	0.734460	-4.385997	0.330423	2294.1481	3129.3622	3146.0635
	H	-1.632960	-3.955656	0.587428	3157.5280	3159.4054	3160.9427
	H	-3.574007	-2.430832	0.464676	3164.6881	3170.6045	3177.0317
	H	-0.948269	0.847322	-0.330725	3179.4161	3186.5586	3194.7235
	H	-5.285996	2.811355	-0.702505	3217.9769	3235.5237	3238.2050
	H	-7.125699	0.421755	-0.104340			
	H	-7.615099	2.163156	-0.505180			
	C	2.181969	-0.663056	-0.081437			
	C	3.561744	-0.703996	0.296235	-105.0790	12.0728	24.5419
	C	1.623986	-1.864897	-0.589710	30.4544	61.7739	81.4489
	C	1.469767	0.604301	-0.022151	86.7955	132.1877	165.3175
	C	4.257198	-1.935628	0.298213	188.4489	214.8102	228.5510
	C	4.250456	0.509215	0.595056	260.8715	280.9923	325.8026
	C	2.335358	-3.046409	-0.610734	360.7621	378.7928	411.9825
	C	2.237606	1.784785	0.125709	438.5878	440.9086	477.3040
	C	3.654561	-3.096508	-0.127875	513.4730	518.2067	526.4785
	C	3.626627	1.707069	0.450538	547.4696	558.7732	577.3347
	C	0.025779	0.746139	-0.101214	593.2052	625.7803	630.3823
	C	1.634330	3.067430	-0.046517	674.4013	677.4068	686.4500
	C	-0.540391	2.044826	-0.316483	703.1227	717.8997	749.1750
	C	0.309525	3.190811	-0.320797	754.7510	760.0701	782.2078
	C	-1.941489	2.206337	-0.447796	805.5357	824.9241	829.1555
	C	-2.808664	1.139038	-0.311994	842.8189	855.6981	877.9572
	C	-0.895152	-0.322477	0.127877	894.6640	896.7851	917.9142
	C	-2.227974	-0.081232	0.003494	958.0370	959.1133	966.9252
TS **[i1]-[i3]**	C	-3.965464	-1.960005	0.545977	975.0852	982.4510	984.2681
	C	-5.056712	-1.711720	-0.206661	1000.9222	1012.4940	1057.4619
	C	-6.132060	-0.881173	0.196211	1077.8095	1112.7003	1123.5676
	C	-7.061933	-0.178496	0.507948	1147.4810	1171.0142	1175.1239
	H	0.636839	-1.851820	-1.025820	1183.7256	1205.5656	1223.8430
	H	5.294432	-1.941060	0.616754	1235.4113	1245.9022	1266.1166
	H	5.295013	0.457976	0.883067	1305.4496	1309.6385	1345.4621
	H	1.876613	-3.938439	-1.022437	1352.0497	1369.1097	1394.8037
	H	4.202207	-4.031960	-0.130225	1409.6505	1435.6794	1440.6885
	H	4.169195	2.633879	0.603599	1451.6548	1471.7630	1501.7910
	H	2.267079	3.945535	0.025260	1529.9233	1545.9937	1589.2275
	H	-0.133198	4.166415	-0.490291	1604.0112	1612.5906	1635.7065
	H	-2.330905	3.202183	-0.637045	1647.7344	1665.1571	2183.6016
	H	-3.881186	1.258921	-0.412838	3140.7042	3151.8414	3156.0524
	H	-0.536850	-1.288089	0.455196	3157.0480	3159.0807	3160.6037
	H	-3.202671	-2.644358	0.198945	3169.2096	3176.4002	3178.7545
	H	-3.881278	-1.589291	1.559199	3179.9491	3185.9154	3196.4620
	H	-5.130695	-2.142687	-1.201658	3226.1540	3248.8228	3475.8164
	H	-7.878993	0.436667	0.794946			
	C	1.871112	-0.748707	-0.186757	-196.8272	5.3687	16.6543
	C	3.112121	-1.109440	0.428363	38.0772	51.6232	77.6764
	C	1.271178	-1.720545	-1.029264	80.1097	105.7963	133.4034
	C	1.354719	0.599017	-0.001030	182.1413	214.1682	230.4630
	C	3.604593	-2.429615	0.304821	260.3498	279.8177	321.7791
	C	3.885051	-0.116048	1.099930	331.6059	378.7735	412.4255
	C	1.790980	-2.991276	-1.160922	437.2512	441.1943	477.0330
	C	2.232787	1.572049	0.535011	506.3166	514.2512	526.3402
	C	2.949877	-3.367180	-0.459757	543.8369	561.3814	577.7224
TS **[i2]-[i4]**	C	3.488243	1.182918	1.094675	593.8013	626.1638	643.2340
	C	0.001218	1.018392	-0.325226	669.6461	675.5987	688.9031
	C	1.875780	2.954595	0.524142	695.3558	704.6005	752.4695
	C	-0.306901	2.417509	-0.367507	757.6847	759.9079	779.3383
	C	0.678506	3.368203	0.033372	806.7105	824.6132	827.8666
	C	-1.603942	2.857070	-0.728063	847.3777	854.7675	880.7395
	C	-2.623084	1.961262	-0.989317	898.2709	901.2808	940.0497
	C	-1.092143	0.117904	-0.507533	952.4492	954.7363	965.8138
	C	-2.314752	0.614675	-0.840386	974.1874	981.7906	1001.0183

	C	-4.162516	-1.062270	-1.139077	1001.1760	1012.2661	1056.3505
	C	-4.517380	-1.452604	-0.045155	1076.1058	1111.6994	1123.0162
	C	-4.838779	-1.875984	1.265284	1147.0775	1170.7845	1174.8593
	C	-5.753672	-1.290889	2.052318	1183.6509	1205.6828	1224.0540
	H	0.415170	-1.451619	-1.628729	1235.3688	1246.1927	1265.5678
	H	4.533645	-2.681752	0.805534	1309.2678	1316.0491	1345.5828
	H	4.820898	-0.409336	1.563528	1352.7355	1368.7700	1394.7045
	H	1.308948	-3.698324	-1.826771	1408.7938	1440.2589	1441.0235
	H	3.343342	-4.372906	-0.553484	1451.6427	1471.6056	1500.5427
	H	4.110837	1.951990	1.539397	1529.8704	1545.4963	1589.1436
	H	2.596792	3.673308	0.898658	1609.7150	1635.6403	1642.4637
	H	0.431046	4.423519	-0.008465	1647.8521	1665.3851	2116.9811
	H	-1.793437	3.925539	-0.771633	3134.8333	3147.7470	3149.0881
	H	-3.615667	2.301047	-1.263092	3156.3284	3158.3195	3159.8296
	H	-0.966927	-0.939577	-0.325253	3169.1935	3172.9960	3175.8307
	H	-4.041611	-0.879519	-2.179012	3178.2688	3185.5699	3201.8407
	H	-4.291603	-2.740944	1.632614	3228.7270	3238.1570	3458.7711
	H	-6.317619	-0.427151	1.721413			
	H	-5.951794	-1.668490	3.047752			
	C	1.628273	-0.917681	-0.135347			
	C	2.906009	-1.429275	0.257540	-549.4400	31.8828	55.9790
	C	0.722250	-1.841852	-0.719005	60.3551	83.7511	90.7434
	C	1.371284	0.507629	-0.014518	124.8739	150.5741	176.8923
	C	3.156535	-2.820387	0.201625	204.8063	234.1915	267.7564
	C	3.945524	-0.526468	0.630278	285.4775	313.3143	315.0433
	C	1.005705	-3.189139	-0.795929	352.6183	362.0083	388.7325
	C	2.478975	1.360772	0.202158	414.5372	433.8347	452.4023
	C	2.218915	-3.694898	-0.296351	470.9277	475.0489	496.5573
	C	3.755121	0.815785	0.540504	533.0458	536.8443	548.4063
	C	0.053929	1.121851	-0.101558	576.7657	588.0589	620.0504
	C	2.335648	2.777327	0.082184	626.6111	639.2966	679.3091
	C	-0.041253	2.540579	-0.270455	692.3889	697.9533	709.7212
	C	1.134555	3.342775	-0.209846	753.6676	758.7729	767.1883
	C	-1.313879	3.139476	-0.411734	798.9971	810.0963	823.1339
	C	-2.465215	2.399186	-0.315836	836.4393	842.9978	852.9396
	C	-1.154761	0.412295	0.076943	866.4732	885.1299	916.0330
	C	-2.403150	1.013524	-0.032124	929.1621	964.2181	968.8936
TS **[i3]-p3**	C	-3.663275	0.281418	0.149338	977.1653	983.3704	990.0166
	C	-3.813754	-1.069646	0.213330	991.2661	1005.7940	1036.7574
	C	-5.066275	-1.713108	0.303342	1043.6177	1068.8388	1126.5989
	C	-6.122232	-2.292701	0.379604	1161.9328	1173.1278	1180.3269
	H	-0.189844	-1.481302	-1.170457	1185.0870	1199.0683	1213.5585
	H	4.123473	-3.183623	0.533777	1232.8729	1238.9521	1256.2879
	H	4.905873	-0.932421	0.929430	1282.0784	1302.6590	1313.4415
	H	0.293881	-3.858828	-1.265333	1332.4068	1353.9378	1370.1898
	H	2.427790	-4.757482	-0.342845	1386.9456	1398.1036	1430.3723
	H	4.567621	1.503701	0.748506	1450.8152	1462.0983	1474.6596
	H	3.219647	3.393677	0.205852	1522.8623	1538.1648	1552.6044
	H	1.042275	4.415372	-0.341872	1589.0144	1608.3666	1634.6210
	H	-1.366906	4.211697	-0.568046	1647.3732	1649.9767	1664.5566
	H	-3.432732	2.879048	-0.415712	2180.8622	3145.9502	3157.7784
	H	-1.105954	-0.624547	0.370972	3158.4951	3159.8389	3161.0498
	H	-3.934055	0.763543	2.175716	3162.0943	3170.2643	3176.8550
	H	-4.565755	0.879689	0.072014	3178.1489	3179.9637	3186.7386
	H	-2.942982	-1.718800	0.215290	3212.3057	3230.6544	3476.2423
	H	-7.055918	-2.794511	0.447859			
	C	-1.426916	0.737638	-0.097604	-1725.4322	28.1825	61.1102
	C	-2.769852	1.152276	0.171102	65.9332	75.5570	123.5347
	C	-0.507811	1.747655	-0.473950	144.8305	169.5902	210.3276
	C	-1.097637	-0.677334	-0.044945	217.4429	251.9788	269.3580
	C	-3.096148	2.528419	0.173818	297.5547	350.2327	379.0390
	C	-3.785992	0.173381	0.379857	399.4588	416.9502	437.6258
TS **[i3]-[i8]**	C	-0.856741	3.081823	-0.487696	458.3068	469.5907	486.3615
	C	-2.164003	-1.603691	0.048804	525.5088	529.1091	534.7779
	C	-2.155824	3.484739	-0.132716	540.8118	564.5802	588.7077
	C	-3.500215	-1.149741	0.271661	606.0610	618.6601	645.2150
	C	0.254929	-1.207023	-0.072845	665.3312	681.0389	691.0470
	C	-1.924351	-3.005958	-0.072895	720.5167	744.6680	752.5442
	C	0.458085	-2.624334	-0.223969	764.1781	789.4582	807.8406
	C	-0.669858	-3.495572	-0.250698	813.8824	834.0892	848.0397

	C	1.769077	-3.158924	-0.286144	856.0469	859.8029	885.6221
	C	2.888093	-2.370444	-0.142889	899.8599	947.6878	958.5524
	C	1.443030	-0.478430	0.110894	966.5212	972.6494	982.0077
	C	2.716164	-0.992831	0.096291	984.2195	1001.6939	1020.4141
	C	3.798190	0.030861	0.373047	1051.0064	1067.1179	1076.0360
	C	3.040673	1.298334	0.823045	1117.1437	1155.3611	1171.7496
	C	3.308368	2.527283	0.155160	1177.3813	1183.7885	1185.9478
	C	3.505339	3.561293	-0.437395	1205.2119	1211.1132	1235.1543
	H	0.482096	1.470988	-0.800160	1239.5285	1250.0848	1285.0926
	H	-4.117149	2.815609	0.403014	1286.3826	1309.4841	1343.8035
	H	-4.797581	0.507884	0.583953	1356.4828	1360.7779	1374.5163
	H	-0.121163	3.819355	-0.787106	1395.5210	1406.7479	1443.6917
	H	-2.420552	4.536029	-0.131971	1453.5797	1469.1780	1484.7205
	H	-4.283109	-1.893658	0.373590	1521.0157	1528.9806	1548.9397
	H	-2.776544	-3.676002	-0.034855	1581.6243	1630.7417	1640.2833
	H	-0.501292	-4.560523	-0.371127	1648.3730	1666.5307	1690.4042
	H	1.874647	-4.229876	-0.423974	2162.2014	3034.5675	3065.0208
	H	3.880918	-2.807691	-0.178303	3088.5470	3153.6727	3156.1016
	H	1.870101	0.856195	0.518831	3157.7249	3159.5491	3172.2804
	H	4.500675	-0.310420	1.139629	3173.1059	3175.6248	3178.0979
	H	4.382826	0.235036	-0.528729	3187.1973	3233.4097	3474.6891
	H	2.971454	1.407970	1.906628			
	H	3.695073	4.472596	-0.949022			
TS **[i3]-[i5]**	C	2.111099	-0.665392	-0.093379			
	C	3.512477	-0.663853	0.197960	-1652.4587	28.8689	61.9177
	C	1.551986	-1.896158	-0.526331	76.4736	79.1970	128.0825
	C	1.374216	0.588000	-0.034254	133.9881	167.5335	203.8869
	C	4.234662	-1.880152	0.200530	232.9040	259.3802	271.5706
	C	4.190989	0.573483	0.406975	309.9299	315.1038	382.8927
	C	2.287584	-3.062450	-0.550900	398.9959	408.1611	426.6440
	C	2.124507	1.787303	0.013171	442.5303	471.3278	492.9776
	C	3.634214	-3.067835	-0.147285	519.5037	528.2128	538.8241
	C	3.532402	1.751338	0.252978	543.7338	589.2467	593.5605
	C	-0.077548	0.694361	-0.021460	603.9617	623.2475	641.2616
	C	1.484544	3.049214	-0.178510	668.0920	678.2021	704.4087
	C	-0.678127	1.974730	-0.265616	709.7328	749.9179	757.0401
	C	0.143410	3.134823	-0.377845	763.0297	800.1808	804.7909
	C	-2.094283	2.104101	-0.308129	808.6284	825.9344	844.8673
	C	-2.849092	1.001194	-0.050341	846.1221	879.0684	884.6252
	C	-0.938498	-0.384069	0.321540	898.3021	917.9376	950.4162
	C	-2.311197	-0.238658	0.305555	965.3629	972.5151	980.4506
	C	-3.367748	-1.272668	0.644133	982.3577	1001.7456	1023.8378
	C	-5.820869	-0.995306	-0.013407	1026.1678	1067.2869	1074.7163
	C	-6.763979	-1.399656	-0.649156	1123.9211	1165.1733	1169.9911
	C	-4.698741	-0.490041	0.706286	1179.6445	1187.4486	1190.8442
	H	0.540229	-1.918838	-0.901699	1203.0210	1227.6198	1232.0749
	H	5.289276	-1.852397	0.454251	1243.4262	1259.7002	1273.3236
	H	5.252125	0.554901	0.631191	1297.5010	1310.8062	1341.5900
	H	1.825733	-3.977569	-0.904284	1361.5549	1365.3909	1374.7363
	H	4.202115	-3.991140	-0.150990	1398.0429	1404.5607	1439.6900
	H	4.062137	2.694576	0.333486	1452.3826	1469.7504	1481.1113
	H	2.101326	3.941590	-0.185775	1508.6940	1530.4308	1548.3428
	H	-0.330795	4.092076	-0.565667	1589.6560	1623.5858	1638.1928
	H	-2.529191	3.077497	-0.511382	1647.6406	1662.4677	1664.7099
	H	-0.514730	-1.319024	0.660185	2168.3478	3038.1704	3067.2864
	H	-3.419704	-2.040943	-0.132482	3083.9182	3156.2794	3157.3989
	H	-3.160778	-1.783938	1.588878	3159.0840	3160.5709	3169.3480
	H	-7.595687	-1.760983	-1.202245	3176.3031	3178.5476	3185.8508
	H	-4.255966	0.589594	0.177469	3198.3513	3224.8503	3475.3519
	H	-4.958138	-0.159254	1.713976			
TS **[i4]-p4**	C	-1.655394	0.946775	-0.136124	-613.9326	27.1555	36.8705
	C	-2.925271	1.485840	0.245669	54.2620	79.9883	97.0150
	C	-0.725658	1.850786	-0.713274	103.9500	118.6694	163.9560
	C	-1.429258	-0.484115	-0.009562	178.0949	205.9814	256.4966
	C	-3.147699	2.881233	0.182769	261.3933	281.1830	320.8393
	C	-3.986233	0.606677	0.615147	342.2735	377.9927	402.3888
	C	-0.981166	3.203368	-0.795942	420.5235	443.4303	445.6682
	C	-2.556634	-1.312494	0.205699	479.3098	491.2943	510.7717
	C	-2.188502	3.735091	-0.310127	535.5808	538.1142	554.9654
	C	-3.823336	-0.739331	0.533618	570.9438	587.3245	629.6624

	C	-0.126645	-1.128592	-0.088108	639.9399	653.8993	690.1093
	C	-2.443496	-2.731851	0.096217	694.1183	707.7075	712.8329
	C	-0.060508	-2.549633	-0.244683	758.1089	766.4201	784.3139
	C	-1.253169	-3.325673	-0.184170	802.9791	810.4516	831.4971
	C	1.198595	-3.182303	-0.380262	840.4563	862.0788	875.3314
	C	2.370472	-2.477025	-0.288441	885.4310	934.2641	937.6248
	C	1.099793	-0.445059	0.084820	952.4928	965.6225	971.7011
	C	2.329106	-1.086877	-0.016947	978.7283	984.2088	994.0995
	C	3.536917	-0.338106	0.158172	1000.3083	1006.4390	1035.6847
	C	4.445017	0.475081	0.092606	1067.0556	1103.0787	1129.5124
	C	5.567666	1.329554	0.075197	1160.2945	1173.1324	1180.4369
	C	5.596809	2.564482	0.601030	1184.9280	1209.8078	1230.7794
	H	0.185411	1.473428	-1.152005	1237.6540	1249.4997	1270.4789
	H	-4.109939	3.264715	0.505710	1287.3319	1315.5264	1326.3889
	H	-4.939876	1.034244	0.905559	1346.9734	1365.3221	1385.2376
	H	-0.249907	3.856902	-1.258107	1396.1200	1420.6441	1444.2938
	H	-2.375637	4.801523	-0.361838	1451.2741	1460.7611	1475.9769
	H	-4.651039	-1.409354	0.740058	1519.9560	1538.1457	1551.3560
	H	-3.341317	-3.328042	0.219245	1586.5760	1630.3980	1640.3135
	H	-1.183511	-4.400970	-0.307510	1647.7293	1650.1043	1664.3852
	H	1.222472	-4.256489	-0.529831	2218.0057	3130.6599	3147.3108
	H	3.328434	-2.973434	-0.377785	3157.7332	3159.6291	3161.1985
	H	1.101512	0.598683	0.355751	3165.8933	3170.5576	3177.2794
	H	4.281002	-1.425068	1.689760	3179.6575	3186.5576	3197.0897
	H	6.458265	0.935802	-0.409598	3218.1082	3238.1103	3238.9064
	H	4.731779	2.992427	1.093205			
	H	6.493915	3.168674	0.547571			
	C	1.573450	-0.413971	-0.193688			
	C	2.971279	-0.434548	0.112320	-458.9975	55.7825	58.0577
	C	1.017174	-1.589500	-0.756139	74.7196	105.5829	119.2246
	C	0.823624	0.816639	-0.011914	151.5376	181.7647	209.1575
	C	3.706961	-1.632901	-0.041031	247.3130	264.5522	298.4216
	C	3.626468	0.769675	0.506204	326.0742	339.6059	371.8065
	C	1.764812	-2.735308	-0.925888	393.9201	430.0377	438.5088
	C	1.553064	2.006208	0.227051	451.0851	473.9199	491.8052
	C	3.116952	-2.771072	-0.540819	523.0117	528.2767	535.8380
	C	2.951874	1.949159	0.511913	573.8679	586.4356	603.6050
	C	-0.623937	0.915123	-0.103221	634.4808	670.1354	676.7104
	C	0.907472	3.278201	0.161065	680.4770	701.7174	723.5590
	C	-1.220637	2.211976	-0.260624	748.7975	762.7195	769.7439
	C	-0.414093	3.380877	-0.139399	781.3171	799.2947	812.7634
	C	-2.613846	2.312748	-0.479823	827.9694	835.4240	851.8183
	C	-3.422541	1.202904	-0.465301	861.6981	882.7619	885.6787
	C	-1.530760	-0.156104	0.012117	944.3683	955.4747	963.6518
	C	-2.891065	-0.077023	-0.156896	969.1224	976.2348	979.9466
TS **[i8]-[i10]**	C	-3.878846	-1.215747	0.059094	995.1663	1008.7564	1025.1730
	C	-2.109449	-2.588300	1.041939	1049.0401	1066.3697	1114.3776
	C	-1.137273	-1.932763	1.399260	1156.7436	1167.2468	1177.4381
	C	-3.281782	-2.635501	0.167601	1182.5499	1184.3675	1200.8449
	H	-0.014688	-1.580055	-1.073983	1209.6841	1228.0996	1238.7194
	H	4.760380	-1.629178	0.219277	1243.5045	1258.7901	1295.5432
	H	4.683537	0.733645	0.747462	1333.5330	1341.5284	1358.6470
	H	1.305429	-3.612746	-1.366782	1361.9672	1378.8609	1391.6038
	H	3.694889	-3.680092	-0.663735	1398.5677	1442.1107	1452.2696
	H	3.465384	2.876725	0.741973	1465.3718	1471.3615	1480.1462
	H	1.508513	4.167532	0.317930	1505.7776	1529.5022	1543.9972
	H	-0.886034	4.351988	-0.246846	1576.2285	1626.7880	1641.7599
	H	-3.042415	3.296152	-0.641398	1647.7779	1663.8437	2024.9316
	H	-4.490550	1.306619	-0.634868	3012.6497	3019.8741	3049.5809
	H	-4.437398	-1.003482	0.978633	3059.3129	3144.1633	3155.0672
	H	-4.613500	-1.208100	-0.753055	3156.6861	3158.5372	3169.6093
	H	-0.249714	-1.658458	1.921779	3170.3799	3174.5621	3177.0791
	H	-2.970489	-2.996797	-0.819540	3184.6513	3214.7024	3424.6886
	H	-4.046749	-3.328385	0.530223			
	C	-1.627959	-0.413816	-0.221800	-453.0873	54.1396	63.8185
	C	-3.014620	-0.403204	0.133163	91.2977	103.5367	126.9684
TS **[i8]-[i9]**	C	-1.127424	-1.590294	-0.835290	145.6392	182.7965	206.5150
	C	-0.835351	0.787397	-0.024912	263.8186	271.6841	290.8217
	C	-3.792187	-1.573426	-0.032844	340.9449	358.0244	367.4698
	C	-3.616802	0.803276	0.597210	400.5113	428.6298	442.0749

	C	-1.914881	-2.707994	-1.011505	460.1486	477.0993	495.0545
	C	-1.514652	1.985161	0.300287	517.2415	533.6358	537.2911
	C	-3.255391	-2.713421	-0.584918	561.5967	598.2082	626.9897
	C	-2.903240	1.959342	0.632827	631.5115	670.8529	681.1935
	C	0.607811	0.847561	-0.185186	694.9220	700.8823	721.5709
	C	-0.827099	3.237613	0.275718	750.1422	763.7010	778.9777
	C	1.247602	2.130637	-0.292883	791.9456	792.9746	812.6633
	C	0.485145	3.315105	-0.067752	828.8454	834.9453	855.4713
	C	2.632053	2.200705	-0.564087	864.2486	879.5700	883.9603
	C	3.400169	1.063238	-0.671721	933.5320	951.0386	964.3947
	C	1.475894	-0.256265	-0.196786	970.2848	975.4075	980.9281
	C	2.828620	-0.211587	-0.449933	987.0862	996.8108	1018.0597
	C	3.682104	-1.458607	-0.436975	1049.7708	1066.5145	1115.9848
	C	2.317093	-2.292074	1.413350	1154.4907	1168.2707	1173.5113
	C	1.159502	-1.890574	1.324199	1180.3668	1184.0661	1201.0533
	C	3.695044	-2.172826	0.953634	1210.5314	1219.8311	1238.7859
	H	-0.104392	-1.605215	-1.183730	1243.1711	1262.6869	1297.5031
	H	-4.835480	-1.546079	0.264170	1315.0714	1337.1497	1355.9336
	H	-4.665706	0.789824	0.873677	1361.2486	1373.7315	1393.0750
	H	-1.497147	-3.585550	-1.491954	1398.8044	1437.7509	1452.1135
	H	-3.865372	-3.600147	-0.715194	1465.7253	1477.2132	1489.1016
	H	-3.377564	2.890691	0.923639	1510.3112	1526.5924	1544.8900
	H	-1.390924	4.136001	0.503326	1575.8494	1625.2193	1637.0467
	H	0.985370	4.275532	-0.135936	1647.6031	1664.3242	2015.0031
	H	3.089884	3.178358	-0.669646	3027.9998	3035.8869	3063.1516
	H	4.461150	1.139823	-0.890306	3082.5999	3148.3894	3155.3214
	H	3.300163	-2.176245	-1.168705	3157.0620	3158.9341	3169.3005
	H	4.709090	-1.215047	-0.721178	3171.8393	3174.9295	3177.3013
	H	0.121282	-1.820538	1.556843	3184.3699	3200.2502	3414.6790
	H	4.276518	-1.590858	1.677040			
	H	4.184542	-3.146229	0.855192			
	C	2.074511	-0.495007	-0.109079			
	C	3.427537	-0.337137	0.330458	-369.2873	42.1225	56.7181
	C	1.733711	-1.747124	-0.684294	82.0840	104.8340	115.0446
	C	1.170092	0.643075	-0.042227	152.5775	176.0198	226.3611
	C	4.305364	-1.446386	0.325577	238.1245	279.1822	296.9088
	C	3.907052	0.955596	0.697005	323.9820	343.2785	379.4457
	C	2.620514	-2.803021	-0.711041	396.4277	418.3597	437.3748
	C	1.741309	1.921310	0.169584	456.0620	475.9755	482.3495
	C	3.909680	-2.668434	-0.166668	524.8970	528.2761	540.6251
	C	3.111032	2.047020	0.555900	568.3555	591.7184	625.5858
	C	-0.275926	0.563056	-0.180864	638.0380	657.2385	669.6506
	C	0.955562	3.101268	0.001163	692.8342	708.1247	718.1252
	C	-1.018191	1.767254	-0.393581	739.5495	757.1101	761.9141
	C	-0.359958	3.029721	-0.333201	792.4136	799.8169	809.1017
	C	-2.427081	1.699685	-0.576126	828.7308	844.3148	854.3858
	C	-3.051845	0.495243	-0.491258	871.3152	873.6553	882.9993
	C	-1.018907	-0.636448	-0.013144	919.4296	934.2929	964.1430
	C	-2.396659	-0.699210	-0.161492	966.7699	974.9411	980.8272
TS **[i5]-[i6]**	C	-3.144594	-2.005504	0.010734	993.2133	1002.1818	1020.2263
	C	-5.192606	-0.788124	0.580359	1033.8784	1067.1765	1125.6542
	C	-5.344206	0.285570	0.020335	1164.8423	1169.8552	1181.5314
	C	-4.356444	-1.916016	0.980744	1190.2998	1195.2947	1202.0312
	H	0.775736	-1.867864	-1.166748	1217.5189	1231.0635	1235.3631
	H	5.316660	-1.304320	0.692375	1246.4622	1272.4873	1308.4209
	H	4.934004	1.055439	1.031741	1326.1203	1336.9780	1354.5170
	H	2.324726	-3.737314	-1.175110	1369.0763	1374.3897	1396.2706
	H	4.596332	-3.507227	-0.173807	1402.3640	1438.5367	1452.3125
	H	3.496154	3.040746	0.758778	1464.8334	1476.4240	1481.4905
	H	1.441987	4.063212	0.123944	1499.7794	1529.4164	1545.2933
	H	-0.941300	3.930138	-0.500507	1583.8923	1613.2237	1636.7434
	H	-2.974410	2.621956	-0.749026	1647.4840	1663.2668	2068.1156
	H	-0.504800	-1.536325	0.294152	3023.5989	3027.8260	3060.8288
	H	-3.524777	-2.329099	-0.964387	3075.7503	3142.6556	3155.8529
	H	-2.460535	-2.781214	0.364936	3157.7002	3159.3969	3168.3791
	H	-5.777125	1.180484	-0.361839	3175.2614	3177.5793	3185.0619
	H	-4.011754	-1.767471	2.009955	3196.0947	3224.8920	3435.4817
	H	-4.910578	-2.859454	0.962247			
TS **[i9]-[i11]**	C	-1.590804	-0.375001	-0.176477	-1663.9030	61.5241	71.2085
	C	-2.968720	-0.333824	0.203244	85.8868	114.5769	127.0480

	C	-1.142672	-1.531645	-0.862179	174.0576	197.8934	239.4679	
	C	-0.757821	0.798651	0.031975	261.2728	297.4943	311.9123	
	C	-3.779687	-1.480230	0.030267	344.1862	393.0600	417.6840	
	C	-3.535899	0.891001	0.664529	440.4403	454.6591	459.2317	
	C	-1.965096	-2.619878	-1.056790	487.7157	496.7520	503.6751	
	C	-1.423380	2.026707	0.273636	539.7350	543.7924	560.1709	
	C	-3.287168	-2.612858	-0.575784	600.0806	609.6216	621.1664	
	C	-2.805968	2.037471	0.632068	663.5665	669.0287	692.3149	
	C	0.693148	0.821597	-0.067299	704.0380	733.7106	755.3709	
	C	-0.729728	3.263858	0.115765	759.4066	766.2746	779.9052	
	C	1.319450	2.073246	-0.362708	787.4462	804.7403	817.2769	
	C	0.567889	3.284030	-0.286240	835.4873	850.6157	855.6518	
	C	2.699982	2.118722	-0.653945	880.9552	895.3183	918.7591	
	C	3.480435	0.989568	-0.550502	941.6703	954.1255	961.5508	
	C	1.557078	-0.296382	0.222638	968.6022	978.1746	986.1681	
	C	2.935676	-0.204395	-0.057722	994.4389	1048.0388	1059.9883	
	C	3.881630	-1.339342	0.317984	1069.4383	1095.5956	1149.1076	
	C	1.786518	-2.663227	0.733400	1169.8732	1174.0218	1182.2963	
	C	1.120643	-1.479890	0.954306	1186.1272	1194.4386	1209.3682	
	C	3.149298	-2.662899	0.372493	1212.6086	1229.8836	1236.7406	
	H	-0.142328	-1.552941	-1.266270	1241.4594	1255.2288	1287.7402	
	H	-4.814381	-1.435246	0.354022	1299.1144	1320.0786	1344.9340	
	H	-4.577899	0.904045	0.966036	1358.3333	1371.7093	1385.6465	
	H	-1.588469	-3.484522	-1.590992	1396.6705	1402.5037	1428.9372	
	H	-3.921956	-3.480597	-0.715317	1447.9436	1450.7553	1468.1203	
	H	-3.261323	2.989343	0.884304	1468.9343	1522.6723	1525.6936	
	H	-1.279461	4.186924	0.265534	1550.7662	1579.0111	1608.0971	
	H	1.073500	4.221465	-0.491479	1634.1945	1647.4543	1661.3758	
	H	3.143155	3.068880	-0.931946	2099.6954	2974.3308	3045.2825	
	H	4.542114	1.040557	-0.770149	3125.5902	3153.7628	3155.8392	
	H	4.711029	-1.392559	-0.394410	3157.9880	3159.5537	3171.6066	
	H	4.340652	-1.113682	1.291732	3173.5930	3175.7974	3178.5753	
	H	0.245188	-1.421561	1.588151	3183.6867	3185.9554	3228.9832	
	H	2.717241	-3.217635	1.488785				
	H	3.584110	-3.544149	-0.093955				
	C	1.586896	-0.371715	-0.176133	-1520.7852		59.8379	70.1530
	C	2.965009	-0.328366	0.198989	84.3903	117.4559	128.2184	
	C	1.137791	-1.532163	-0.855045	172.0656	200.9439	239.9249	
	C	0.753362	0.803492	0.030580	261.8014	298.3876	313.2714	
	C	3.775207	-1.476349	0.031333	345.8708	392.9239	417.3023	
	C	3.533857	0.899295	0.652226	439.5639	449.5318	470.5443	
	C	1.958887	-2.621964	-1.045615	478.8265	494.9822	516.6750	
	C	1.420055	2.033572	0.264355	539.6806	543.4783	556.2510	
	C	3.281409	-2.612923	-0.565795	596.8001	610.4077	616.9625	
	C	2.804375	2.045681	0.616784	664.5130	673.2397	686.7246	
	C	-0.695178	0.826008	-0.059804	705.5718	732.9019	752.1999	
	C	0.723744	3.268526	0.110158	756.1877	768.9369	775.5196	
	C	-1.325688	2.073522	-0.352060	786.7234	800.5728	815.9539	
	C	-0.577845	3.286015	-0.281382	837.2030	848.6473	856.1283	
	C	-2.707914	2.112361	-0.647432	881.1724	894.6058	934.4362	
	C	-3.484224	0.978874	-0.553756	942.2981	953.4840	961.9263	
	C	-1.557715	-0.301941	0.229395	965.7466	971.4221	979.0491	
TS **[i10]-[i11]**	C	-2.937792	-0.215060	-0.065886	994.8312	1042.0476	1060.8654	
	C	-3.871981	-1.351340	0.313667	1065.1841	1095.4358	1149.1713	
	C	-1.809454	-2.708036	0.897040	1169.6899	1174.3192	1182.3006	
	C	-1.121166	-1.460555	0.962496	1188.1915	1193.7461	1209.1035	
	C	-3.137477	-2.662125	0.442336	1226.0220	1231.9552	1239.3325	
	H	0.138747	-1.550626	-1.264061	1243.4364	1258.4689	1287.1919	
	H	4.810379	-1.429864	0.353128	1290.6607	1330.5159	1353.6932	
	H	4.576643	0.913398	0.950720	1356.3671	1367.1781	1384.5811	
	H	1.582212	-3.489362	-1.575233	1395.1540	1398.0944	1435.1678	
	H	3.915134	-3.482123	-0.699970	1437.5237	1449.7841	1456.9251	
	H	3.260688	2.998433	0.863639	1467.8940	1519.9434	1523.8437	
	H	1.272558	4.192805	0.255385	1548.2991	1573.7121	1602.4145	
	H	-1.086478	4.222203	-0.484536	1632.4147	1647.5059	1660.4441	
	H	-3.153990	3.061168	-0.925252	2113.6210	2957.8831	3047.3122	
	H	-4.545423	1.026935	-0.776065	3120.8683	3154.9942	3156.9589	
	H	-4.334386	-1.122323	1.287492	3159.1991	3160.5890	3172.1822	
	H	-4.696436	-1.424710	-0.402447	3174.5152	3176.6971	3179.3516	
	H	-0.219444	-1.393332	1.558062	3180.1557	3186.7434	3220.2845	

	H	-2.110016	-3.047357	-0.308121				
	H	-3.695136	-3.584093	0.288545				
	C	2.038163	-0.520823	-0.092759				
	C	3.430185	-0.352200	0.193135	-1700.3862		54.8562	61.9964
	C	1.629281	-1.804272	-0.538315	87.1421	117.1408	143.8342	
	C	1.153553	0.632887	-0.014467	171.3200	213.4596	234.4567	
	C	4.294615	-1.471518	0.175989	269.9479	289.2562	322.2147	
	C	3.953996	0.956152	0.416483	344.9542	384.0382	407.2432	
	C	2.500727	-2.872913	-0.580753	421.9041	443.1758	470.2601	
	C	1.752990	1.916168	0.050199	478.1695	497.2564	519.9332	
	C	3.840475	-2.719247	-0.184491	536.9402	545.5283	568.5335	
	C	3.155427	2.047454	0.283505	596.6366	602.8739	635.9964	
	C	-0.294090	0.564510	0.003186	643.3923	689.6827	708.7508	
	C	0.960156	3.092409	-0.110639	711.4726	727.0900	756.6752	
	C	-1.053665	1.759183	-0.205815	761.1036	763.6709	791.9794	
	C	-0.384044	3.015782	-0.295306	804.7791	807.1441	810.7425	
	C	-2.460701	1.694891	-0.265930	829.2305	841.4296	848.5460	
	C	-3.157010	0.516069	-0.041003	883.3176	898.2262	908.3934	
	C	-1.032495	-0.610381	0.324322	935.7000	944.8722	964.7501	
	C	-2.405631	-0.649767	0.319291	973.3536	980.6693	987.8097	
TS **[i6]-[i7]**	C	-3.170773	-1.880339	0.791455	1004.3042	1022.0691	1066.3096	
	C	-5.131217	-0.825518	-0.379028	1073.5683	1110.2944	1155.6068	
	C	-4.605499	0.411354	-0.089729	1172.1206	1172.9734	1181.8517	
	C	-4.454899	-2.006607	-0.008811	1187.7134	1197.4616	1207.9407	
	H	0.625164	-1.944079	-0.909013	1220.2810	1229.1005	1243.2871	
	H	5.339711	-1.319252	0.424955	1251.2263	1283.8818	1285.7264	
	H	5.010928	1.064180	0.635203	1297.3764	1321.0480	1352.4397	
	H	2.151131	-3.833285	-0.942941	1358.4393	1372.6629	1386.3964	
	H	4.516496	-3.566430	-0.203093	1401.2102	1421.7689	1441.0029	
	H	3.567297	3.046708	0.377177	1450.4342	1458.9801	1467.8952	
	H	1.462276	4.053995	-0.104035	1480.4958	1514.9361	1534.3701	
	H	-0.974665	3.910795	-0.458719	1543.9015	1588.7499	1630.6153	
	H	-3.012315	2.605867	-0.477365	1632.8114	1646.9141	1663.3867	
	H	-0.499930	-1.489976	0.656933	2086.1234	2985.8295	3069.6087	
	H	-2.562354	-2.783786	0.704029	3129.5471	3155.2599	3156.7906	
	H	-3.406153	-1.765316	1.858937	3158.6375	3160.1886	3162.3256	
	H	-5.216579	1.303392	-0.005416	3168.6800	3176.1289	3178.3709	
	H	-5.662328	-1.701827	0.451312	3185.3879	3199.8619	3224.7469	
	H	-4.695951	-2.940625	-0.511079				
	C	-1.599488	-0.391049	-0.189755	-614.2902	64.4063	71.8890	
	C	-2.979403	-0.358040	0.177828	89.2386	119.7419	164.5903	
	C	-1.147302	-1.531160	-0.900284	173.1696	225.3504	240.1634	
	C	-0.766944	0.781455	0.051720	269.5898	279.7282	308.6706	
	C	-3.790829	-1.498124	-0.033435	339.8386	347.5175	401.2336	
	C	-3.552363	0.855159	0.666968	421.4001	430.8477	455.9443	
	C	-1.969195	-2.612492	-1.132739	473.8253	484.0456	500.9000	
	C	-1.439258	2.003821	0.316259	527.0485	537.7712	544.4935	
	C	-3.296466	-2.615416	-0.665328	557.0089	576.5925	613.6277	
	C	-2.825178	2.002161	0.667891	634.8206	658.3497	679.5790	
	C	0.677973	0.813792	-0.047541	691.4373	723.1052	735.5224	
	C	-0.748180	3.241297	0.194787	755.4312	768.5988	782.6559	
	C	1.297405	2.062642	-0.320447	787.9499	797.6326	806.9141	
	C	0.552377	3.269354	-0.208376	821.6653	839.9804	857.4565	
	C	2.681406	2.117828	-0.669802	866.6391	884.7875	900.0322	
TS **[i11]-p2**	C	3.457590	1.001039	-0.663334	937.6128	948.6799	961.6052	
	C	1.562465	-0.316995	0.204167	968.4290	973.4934	980.5162	
	C	2.935881	-0.227495	-0.168762	983.5940	999.0976	1000.6040	
	C	3.796007	-1.347799	0.029675	1047.6943	1059.6087	1082.9569	
	C	1.165610	-1.457500	0.947520	1092.2300	1147.0989	1164.6513	
	C	2.042583	-2.488871	1.224210	1170.8536	1178.6858	1183.9149	
	C	3.360718	-2.450431	0.755091	1185.0014	1207.4299	1222.7462	
	H	-0.139561	-1.548348	-1.289014	1233.3699	1239.1393	1249.4128	
	H	-4.828191	-1.459364	0.282310	1283.4825	1296.0348	1343.6977	
	H	-4.596587	0.858635	0.960574	1352.2698	1362.1483	1375.3223	
	H	-1.590295	-3.461249	-1.690712	1396.6649	1410.4680	1444.0620	
	H	-3.932315	-3.476872	-0.834983	1448.2690	1460.5165	1470.0746	
	H	-3.283691	2.946828	0.940347	1513.8613	1525.8701	1545.7011	
	H	-1.295309	4.161032	0.371267	1552.0033	1585.7467	1619.1331	
	H	1.057666	4.211217	-0.392484	1623.1026	1648.1871	1649.5638	
	H	3.100593	3.079409	-0.946217	1660.0740	3157.1910	3158.9652	

	H	4.499138	1.046106	-0.962390	3159.7601	3161.9095	3166.3569
	H	3.759216	-2.140019	-1.780784	3170.7669	3174.0605	3176.7994
	H	4.849621	-1.230268	-0.195690	3178.3302	3180.3640	3185.8035
	H	0.160109	-1.508908	1.338773	3189.7360	3216.7357	3218.4385
	H	1.706393	-3.328105	1.822376			
	H	4.040757	-3.269154	0.958744			
	C	2.061256	-0.508632	-0.103972			
	C	3.445930	-0.325133	0.214754	-602.5422	56.1996	61.9073
	C	1.682954	-1.788777	-0.589923	90.1569	121.2164	150.8247
	C	1.159823	0.625189	-0.011139	192.8755	215.9640	251.6360
	C	4.330286	-1.429984	0.184206	256.4419	288.9515	310.3155
	C	3.939860	0.981560	0.491068	322.0044	345.7137	400.0493
	C	2.573896	-2.838641	-0.644934	407.4204	419.6062	440.7707
	C	1.730075	1.911124	0.110747	475.8547	499.6234	507.9516
	C	3.904614	-2.673350	-0.218672	523.2941	533.6156	538.6144
	C	3.121872	2.062857	0.379044	570.4186	590.1839	601.2904
	C	-0.298719	0.529930	-0.033279	635.5027	650.7582	663.2392
	C	0.919797	3.085789	-0.046928	713.5809	717.6549	746.4658
	C	-1.073932	1.730376	-0.249604	757.4377	763.8715	780.5972
	C	-0.409965	2.999807	-0.286026	791.2173	806.3220	810.6429
	C	-2.463385	1.660271	-0.337105	817.8217	842.1356	847.9081
	C	-3.160451	0.460660	-0.149971	871.8558	883.4549	903.2796
	C	-1.009826	-0.642502	0.244895	917.0404	927.8432	949.1374
	C	-2.407664	-0.709944	0.194235	966.0316	972.8806	978.9767
TS **[i7]-p1**	C	-3.120132	-1.921420	0.487494	983.2689	996.2913	1003.7999
	C	-4.579085	0.366274	-0.253177	1023.9583	1036.4318	1066.6979
	C	-5.222962	-0.826614	-0.037829	1108.0412	1152.7218	1162.9216
	C	-4.491341	-1.982904	0.318519	1170.9885	1181.4662	1183.3727
	H	0.687905	-1.937063	-0.980849	1194.0830	1212.9451	1229.6047
	H	5.367175	-1.267178	0.459254	1235.7012	1253.8984	1284.4705
	H	4.989454	1.102167	0.736802	1292.9961	1313.2272	1354.6305
	H	2.248477	-3.794835	-1.039170	1355.7754	1373.2701	1383.6349
	H	4.594582	-3.508884	-0.246759	1399.9776	1405.6948	1443.7121
	H	3.512397	3.065804	0.514415	1447.8166	1454.1950	1477.2169
	H	1.410591	4.052119	-0.001224	1507.9401	1522.7811	1541.9841
	H	-1.005184	3.891484	-0.450464	1565.4976	1583.8645	1616.7182
	H	-3.022034	2.572994	-0.520308	1631.2074	1648.3322	1653.6229
	H	-0.481699	-1.529481	0.562829	1668.6357	3155.7840	3157.5589
	H	-2.551746	-2.827776	0.661028	3159.3366	3160.8610	3161.5331
	H	-3.091638	-1.863860	2.500104	3169.3415	3169.5889	3176.8540
	H	-5.142229	1.255116	-0.517414	3178.7707	3179.2259	3186.1456
	H	-6.300472	-0.888444	-0.139563	3190.6942	3206.8512	3227.3671
	H	-5.012992	-2.917778	0.486910			
	C	-1.982297	0.732554	-0.075879	21.2395	24.1016	58.2289
	C	-3.384833	0.869815	0.174265	78.2018	103.1504	122.7830
	C	-1.287085	1.906684	-0.466122	158.5216	178.2157	203.4617
	C	-1.379094	-0.590446	-0.019146	236.9210	269.2056	289.2218
	C	-3.979145	2.153349	0.178895	333.3684	355.0592	388.9071
	C	-4.191881	-0.294757	0.341400	394.9109	419.7895	431.7278
	C	-1.898595	3.142683	-0.488786	445.7084	450.8421	484.2696
	C	-2.248377	-1.708271	-0.010383	492.3126	529.8009	535.0711
	C	-3.250032	3.279060	-0.126708	544.4023	555.7667	589.6542
	C	-3.652114	-1.531690	0.188539	613.2199	633.1937	643.3473
	C	0.051198	-0.848958	0.031263	647.8110	687.8662	700.4169
	C	-1.734451	-3.027288	-0.197489	709.1923	745.6476	757.8593
	C	0.525660	-2.176480	-0.205709	768.7824	798.9641	809.5781
[i3]	C	-0.402795	-3.247507	-0.355037	812.5438	830.1681	840.5845
	C	1.917808	-2.430134	-0.213456	860.9246	877.1623	884.2315
	C	2.826643	-1.442355	0.074994	904.8475	928.0731	964.7478
	C	1.020823	0.118979	0.405520	969.7436	978.4163	982.4000
	C	2.375019	-0.153315	0.434544	988.5607	1001.8693	1022.3462
	C	3.378644	0.905931	0.859951	1037.0449	1067.0950	1128.4118
	C	4.276368	1.335683	-0.270991	1143.0428	1159.4657	1170.8152
	C	5.645898	1.288740	-0.215930	1179.2972	1183.7045	1185.7527
	C	6.865511	1.242296	-0.156578	1200.3158	1219.9078	1235.2628
	H	-0.266495	1.832028	-0.809058	1238.7740	1257.3189	1280.2597
	H	-5.038597	2.229681	0.400518	1294.9944	1326.6578	1351.8436
	H	-5.252136	-0.170812	0.534230	1369.9591	1383.7783	1397.4396
	H	-1.334421	4.011818	-0.808153	1400.2551	1430.9040	1449.8843
	H	-3.720517	4.255610	-0.128798	1461.7501	1472.5383	1477.7575

	H	-4.277303	-2.416790	0.239048	1526.5206	1538.8976	1555.5663
	H	-2.438747	-3.851532	-0.233690	1592.5336	1636.2499	1647.8613
	H	-0.022025	-4.246645	-0.537779	1652.4443	1666.2812	2014.2739
	H	2.257160	-3.438795	-0.425428	3001.7119	3065.2893	3150.6991
	H	3.890009	-1.655989	0.068594	3157.1752	3158.5165	3160.0505
	H	0.692814	1.091764	0.741487	3161.3548	3169.7875	3176.6117
	H	2.831095	1.777568	1.240987	3178.0857	3179.7016	3186.8458
	H	3.991288	0.533553	1.685712	3205.4623	3228.4039	3468.2338
	H	3.804655	1.694853	-1.180917			
	H	7.925971	1.206238	-0.109699			
	C	1.472103	0.861239	0.207059			
	C	2.719012	1.432532	-0.203689	19.4780	39.4353	69.6608
	C	0.568734	1.722519	0.883220	80.3278	103.2524	122.9031
	C	1.245584	-0.561077	0.005766	157.1682	179.2857	210.5676
	C	2.938768	2.823106	-0.066073	226.4332	267.5553	288.2578
	C	3.763235	0.585975	-0.680093	320.9013	354.9035	361.6898
	C	0.822678	3.069124	1.036241	389.8245	422.9993	451.0569
	C	2.364364	-1.365451	-0.316966	465.1563	480.4362	510.4140
	C	2.002297	3.638473	0.525462	526.5091	535.3447	542.6870
	C	3.609632	-0.763688	-0.673704	550.1122	586.2226	587.7526
	C	-0.049969	-1.219218	0.114109	617.3693	638.9182	688.0493
	C	2.266355	-2.790757	-0.287516	690.1791	708.9712	740.1578
	C	-0.096570	-2.649229	0.189775	750.0528	757.3663	765.1666
	C	1.096551	-3.409832	0.019275	787.4072	808.4512	813.5781
	C	-1.341215	-3.297759	0.352458	822.4192	836.6289	845.2333
	C	-2.518757	-2.590904	0.367118	864.1973	884.3718	899.1424
	C	-1.287206	-0.539154	0.050182	935.3694	937.8177	940.5028
	C	-2.506956	-1.190917	0.176699	962.5188	967.7755	975.5575
[i4]	C	-3.795185	-0.470491	0.097759	982.0822	990.3153	1004.7153
	C	-3.973926	0.817592	-0.040450	1036.2228	1068.0129	1086.2453
	C	-4.195422	2.141332	-0.171268	1127.5073	1160.6706	1172.3220
	C	-4.328636	2.830531	-1.375266	1179.8724	1184.3798	1191.3625
	H	-0.319197	1.312847	1.339599	1196.6447	1213.0002	1232.4877
	H	3.882148	3.232228	-0.412542	1238.0580	1255.4454	1276.9145
	H	4.699087	1.037414	-0.991690	1301.6351	1333.1144	1351.6447
	H	0.111745	3.688231	1.571765	1368.1878	1384.5415	1397.1027
	H	2.187373	4.701122	0.633166	1405.9426	1435.9405	1450.5433
	H	4.428383	-1.413833	-0.963142	1459.7056	1476.5381	1490.6030
	H	3.160392	-3.369867	-0.492534	1526.5107	1538.4134	1556.4723
	H	1.039242	-4.491252	0.082016	1589.9130	1633.4741	1647.6087
	H	-1.353725	-4.379436	0.436595	1648.0005	1665.5020	1885.7004
	H	-3.465802	-3.106961	0.484279	3056.6608	3094.0999	3150.3189
	H	-1.304803	0.520027	-0.158462	3156.0548	3156.9382	3158.6799
	H	-4.682356	-1.105499	0.164547	3160.1043	3169.6600	3174.1132
	H	-4.274412	2.716001	0.752414	3176.2630	3178.5856	3185.7921
	H	-4.258569	2.317031	-2.325451	3211.3228	3230.6473	3251.3962
	H	-4.502331	3.898292	-1.381149			
	C	-1.755607	0.896096	-0.063462	20.9817	27.1309	56.9319
	C	-3.117164	1.312026	0.076744	66.0382	86.2301	137.4484
	C	-0.789561	1.912667	-0.257482	141.7460	154.5241	179.9526
	C	-1.436470	-0.519890	-0.002513	236.7652	259.8497	271.9970
	C	-3.443625	2.687015	0.019143	326.8970	340.2527	361.9092
	C	-4.140979	0.338968	0.273610	399.9303	415.9753	417.8330
	C	-1.132168	3.246555	-0.309820	458.0292	467.5431	493.7751
	C	-2.491409	-1.441545	0.193323	511.6699	530.2973	539.4239
	C	-2.473830	3.643923	-0.170396	553.2599	592.8058	614.0117
	C	-3.837460	-0.983522	0.329162	635.1624	666.1809	677.2546
	C	-0.092801	-1.052622	-0.132193	681.5355	695.4415	711.7454
[i8]	C	-2.232840	-2.845518	0.258084	739.9492	746.0956	761.4166
	C	0.132691	-2.471417	-0.065137	768.8525	792.4811	808.4876
	C	-0.975510	-3.344825	0.133369	813.2809	834.9309	836.2980
	C	1.447284	-2.977962	-0.200521	857.4593	880.8906	901.7412
	C	2.529582	-2.150804	-0.394314	953.9014	958.5661	966.6080
	C	1.070157	-0.308488	-0.325982	971.3250	973.6158	982.3236
	C	2.355110	-0.742498	-0.464678	993.8194	1006.2757	1008.1213
	C	3.532057	0.190509	-0.640016	1051.8335	1067.4455	1118.8705
	C	5.318777	1.472149	0.563345	1154.2607	1170.0002	1176.1210
	C	6.264967	2.196377	0.407228	1180.8176	1184.2559	1209.6352
	C	4.165557	0.590644	0.717416	1220.5079	1240.2416	1242.8224
	H	0.251463	1.630070	-0.369436	1261.7048	1288.7695	1294.5942

	H	-4.484057	2.974884	0.128493	1311.5194	1341.7475	1362.6664
	H	-5.166549	0.676962	0.377583	1364.5727	1373.1040	1400.3637
	H	-0.360060	3.992724	-0.460246	1403.7846	1448.6434	1456.3538
	H	-2.738726	4.694297	-0.212591	1466.6627	1476.7498	1498.7916
	H	-4.617573	-1.722304	0.478366	1503.4406	1533.0828	1542.6234
	H	-3.074772	-3.512430	0.409965	1580.0393	1632.2273	1649.4265
	H	-0.794648	-4.413394	0.182862	1650.4145	1668.3215	2221.2532
	H	1.589841	-4.052245	-0.153417	3025.1199	3048.6983	3055.0933
	H	3.526181	-2.568541	-0.503767	3096.4008	3121.8277	3149.5636
	H	4.295649	-0.289124	-1.258328	3157.4501	3159.3990	3161.1150
	H	3.217725	1.096040	-1.162894	3171.7758	3173.7446	3176.9449
	H	7.102294	2.837369	0.279562	3179.4370	3186.9423	3477.9764
	H	4.466103	-0.312975	1.258803			
	H	3.406573	1.081635	1.335577			
	C	-1.818162	0.867495	-0.078652			
	C	-3.173138	1.230170	0.205970	19.8198	42.1695	55.2886
	C	-0.958251	1.909002	-0.514863	81.4904	89.7401	122.2006
	C	-1.430792	-0.533301	-0.008352	148.5408	177.3713	188.9169
	C	-3.556269	2.591736	0.198373	231.1882	273.1849	288.1513
	C	-4.149566	0.212089	0.419298	326.5804	343.4061	366.0330
	C	-1.367051	3.225687	-0.549289	395.6506	409.1491	428.0798
	C	-2.466085	-1.497688	0.044463	444.5670	472.1702	486.2228
	C	-2.667910	3.581539	-0.152802	526.7462	531.0622	548.5695
	C	-3.817717	-1.097049	0.276880	549.6976	591.6528	627.0072
	C	-0.057317	-1.014395	0.009547	636.1418	665.3452	675.2979
	C	-2.174400	-2.883620	-0.133697	676.2206	695.4954	706.6086
	C	0.188793	-2.406072	-0.218573	744.9136	755.2180	760.3557
	C	-0.900657	-3.317696	-0.324685	770.3278	793.2248	808.9366
	C	1.530253	-2.883481	-0.256811	811.9793	831.4667	844.0347
	C	2.523982	-2.001320	0.001244	870.5817	883.0316	894.4295
	C	1.056260	-0.197068	0.344117	919.1696	964.7567	967.1339
	C	2.365250	-0.662576	0.352579	969.5426	977.5950	982.3796
[i5]	C	3.531655	0.218425	0.732772	1002.0017	1009.0660	1018.3519
	C	5.610259	1.337193	-0.107213	1040.8558	1069.0899	1125.7692
	C	6.534653	2.035732	0.211667	1164.6023	1169.1462	1181.4715
	C	4.474766	0.492985	-0.465069	1182.6597	1194.2369	1212.4835
	H	0.026341	1.667377	-0.885265	1229.1079	1234.7032	1245.2618
	H	-4.582920	2.839083	0.447532	1266.4937	1283.5869	1302.5603
	H	-5.170413	0.506303	0.638000	1315.4997	1338.4331	1360.7314
	H	-0.682819	3.988139	-0.904337	1369.5843	1377.1486	1396.1896
	H	-2.977598	4.620242	-0.164072	1400.2489	1437.8806	1452.5145
	H	-4.573547	-1.870567	0.361337	1463.9301	1476.8525	1494.9042
	H	-3.001592	-3.585430	-0.136423	1501.4113	1529.9166	1545.5781
	H	-0.689702	-4.366820	-0.500826	1581.6110	1617.8564	1640.2484
	H	1.716785	-3.933935	-0.455878	1647.7478	1663.5207	2221.5530
	H	0.887610	0.818987	0.672491	3023.4189	3044.0567	3052.4921
	H	3.164320	1.168918	1.126695	3090.6871	3158.0477	3158.8592
	H	4.112105	-0.256463	1.529041	3160.4280	3162.3529	3170.6773
	H	7.355901	2.651415	0.485051	3178.0670	3180.4242	3186.9068
	H	3.906609	0.967230	-1.272749	3198.8952	3226.1590	3476.9764
	H	4.837583	-0.461196	-0.862022			
	C	-1.588146	-0.393687	0.167637	63.1872	73.2836	86.4047
	C	-2.971867	-0.369241	-0.194111	117.5067	147.6835	168.4763
	C	-1.116026	-1.547214	0.843706	200.9870	238.6904	267.5989
	C	-0.773602	0.789363	-0.047010	287.7063	321.2578	343.7794
	C	-3.765473	-1.526450	-0.011967	389.1260	397.0494	415.5350
	C	-3.557968	0.848333	-0.649330	442.4055	459.5324	483.3620
	C	-1.922003	-2.645706	1.048042	496.4862	502.5151	532.3535
	C	-1.454691	2.008884	-0.279629	545.4033	552.5624	564.2764
	C	-3.251057	-2.653846	0.585422	608.7874	614.5937	656.2210
[i10]	C	-2.840259	2.003221	-0.625373	685.0198	691.6739	711.0571
	C	0.679378	0.828379	0.050919	740.4134	756.2370	767.8154
	C	-0.774862	3.254114	-0.113731	783.6077	785.4028	802.7958
	C	1.288071	2.084910	0.369028	812.7760	834.9119	855.8864
	C	0.519417	3.286429	0.296803	860.5552	863.0311	882.6500
	C	2.665190	2.143210	0.665803	902.3280	937.9058	948.3268
	C	3.455206	1.022190	0.560262	956.8788	963.8812	970.6100
	C	1.556966	-0.268066	-0.240471	979.3549	985.4667	995.4072
	C	2.924294	-0.175330	0.054006	1016.8923	1047.8895	1069.5929
	C	3.869030	-1.305707	-0.313474	1073.4889	1150.0530	1168.5542

	C	1.893304	-2.540198	-0.995287	1170.8699	1173.9436	1182.6057
	C	1.117445	-1.472427	-0.994199	1188.7820	1196.3334	1217.9568
	C	3.196723	-2.696417	-0.313347	1229.4629	1237.6615	1242.4905
	H	-0.108868	-1.554490	1.233470	1248.4936	1277.5929	1306.6401
	H	-4.804724	-1.494466	-0.322364	1325.5912	1341.2439	1359.0647
	H	-4.603099	0.849616	-0.939992	1362.0801	1382.9805	1389.5904
	H	-1.529770	-3.505772	1.578815	1406.0505	1443.1317	1450.3539
	H	-3.873359	-3.529266	0.732568	1463.6902	1467.9598	1473.8603
	H	-3.309616	2.949662	-0.872307	1522.8943	1526.9296	1554.1670
	H	-1.334753	4.171703	-0.259113	1581.6853	1617.3194	1637.3995
	H	1.012120	4.228547	0.511926	1647.3053	1661.5135	1684.0870
	H	3.097409	3.095946	0.952350	2988.8502	2999.0710	3057.1185
	H	4.513599	1.077891	0.793485	3059.3449	3155.8585	3157.1652
	H	4.256559	-1.111216	-1.322743	3159.3455	3160.9640	3171.1843
	H	4.731579	-1.305278	0.359610	3174.8587	3176.8820	3178.5392
	H	0.177599	-1.437042	-1.531272	3180.0021	3186.4377	3220.4690
	H	3.038243	-3.057635	0.712479			
	H	3.842648	-3.426671	-0.809114			
	C	-1.620978	-0.406917	-0.187939			
	C	-2.996907	-0.384326	0.202833	60.5803	72.4599	94.3599
	C	-1.174805	-1.538554	-0.918114	110.7395	148.4704	170.2267
	C	-0.789977	0.758339	0.059368	200.8996	233.8469	269.4707
	C	-3.807344	-1.524035	-0.014208	281.8038	316.8027	350.6178
	C	-3.559519	0.815906	0.727752	369.9577	403.3801	414.3677
	C	-1.996935	-2.618433	-1.153486	441.2227	465.0887	482.6106
	C	-1.452204	1.971055	0.365496	486.4337	517.3034	529.0945
	C	-3.318465	-2.630344	-0.669052	544.6693	551.8793	563.3616
	C	-2.828899	1.962797	0.744140	609.3955	624.9437	655.4996
	C	0.659518	0.791208	-0.092183	686.0112	702.8498	711.5533
	C	-0.765169	3.217660	0.237266	741.2013	755.9226	767.6273
	C	1.266654	2.056123	-0.383631	785.1053	792.5665	794.9954
	C	0.512726	3.259033	-0.219407	813.4800	835.1999	853.0667
	C	2.626943	2.118242	-0.744445	856.8479	860.6949	884.2095
	C	3.403988	0.980971	-0.751593	900.1224	935.6087	951.9478
	C	1.539069	-0.321810	0.108247	954.2983	964.0801	970.9982
	C	2.884287	-0.233631	-0.283242	979.0136	980.9565	997.4679
[i9]	C	3.767185	-1.464726	-0.208256	1023.8976	1047.0090	1067.9697
	C	2.086777	-2.352619	1.315551	1073.8323	1150.3563	1169.4297
	C	1.149943	-1.517911	0.904598	1170.9311	1173.8860	1183.0827
	C	3.542981	-2.295224	1.080563	1190.2024	1197.3469	1217.2925
	H	-0.172078	-1.544355	-1.321215	1229.4312	1240.5303	1245.1238
	H	-4.839824	-1.494257	0.318199	1250.0809	1281.3115	1309.0612
	H	-4.598073	0.813942	1.040957	1321.5650	1338.7913	1360.6319
	H	-1.623674	-3.460349	-1.725491	1362.5997	1381.9924	1390.7972
	H	-3.954054	-3.491354	-0.841894	1407.4156	1442.1422	1450.3927
	H	-3.281868	2.900999	1.046813	1467.4693	1470.1817	1480.3893
	H	-1.310886	4.131731	0.445162	1521.7482	1528.6072	1555.2117
	H	1.005987	4.206431	-0.408554	1583.0583	1616.5319	1636.5493
	H	3.057901	3.081432	-0.995412	1647.6369	1662.1176	1686.7008
	H	4.444671	1.033167	-1.054316	2992.6225	3002.4995	3057.0897
	H	3.533402	-2.109208	-1.065739	3066.9040	3156.0036	3156.6620
	H	4.820440	-1.185639	-0.296660	3158.5888	3159.9949	3169.9325
	H	0.123781	-1.626758	1.227683	3174.5224	3176.2784	3178.8807
	H	4.031880	-1.825638	1.945271	3185.2751	3196.3133	3210.7266
	H	3.989186	-3.286966	0.963648			
	C	2.057396	-0.501917	-0.100237	54.0698	60.5808	91.6892
	C	3.427514	-0.322209	0.272398	113.9806	140.3823	176.4143
	C	1.701754	-1.771189	-0.625884	200.6312	235.2587	271.8463
	C	1.147176	0.631583	-0.021996	284.9441	314.7446	330.5106
	C	4.313886	-1.424400	0.256879	383.5519	400.3906	411.6034
	C	3.912360	0.983597	0.581693	427.8837	445.9066	478.9992
	C	2.595611	-2.820962	-0.665037	491.5455	514.6869	536.1300
[i6]	C	1.717137	1.919819	0.129533	541.9846	563.7318	578.1798
	C	3.906793	-2.662288	-0.184025	598.3350	637.1129	644.7234
	C	3.101881	2.065429	0.448337	692.3128	712.8424	715.1647
	C	-0.300766	0.539610	-0.089508	745.5476	759.0816	764.3579
	C	0.914171	3.089249	-0.030022	767.1900	805.8526	810.9232
	C	-1.065742	1.730043	-0.292590	814.1109	829.1399	838.9731
	C	-0.415606	2.999079	-0.295686	850.2073	883.2867	891.5172
	C	-2.471806	1.651414	-0.405682	906.3937	923.2191	931.6986

	C	-3.150200	0.459409	-0.255768	944.6735	964.7687	974.2282
	C	-1.035520	-0.657703	0.129161	978.2221	981.8393	1001.3788
	C	-2.408929	-0.719255	0.046251	1018.8911	1024.3488	1067.6632
	C	-3.151430	-2.032905	0.196908	1102.5328	1155.8036	1171.4566
	C	-5.207645	-0.692691	0.211096	1174.4265	1178.8858	1183.0841
	C	-4.625612	0.378294	-0.298145	1202.3748	1206.5237	1221.5723
	C	-4.560225	-1.872907	0.826140	1231.0523	1242.7774	1250.6538
	H	0.724348	-1.912319	-1.061252	1257.7443	1282.8717	1319.0821
	H	5.339541	-1.264937	0.573082	1322.8779	1345.3584	1355.1463
	H	4.952603	1.099577	0.866437	1371.4460	1382.5714	1396.7030
	H	2.286995	-3.769672	-1.089834	1418.1554	1450.4548	1463.9677
	H	4.599609	-3.495861	-0.200175	1467.0972	1476.5270	1482.7179
	H	3.487762	3.066813	0.607272	1513.8845	1534.5134	1545.6278
	H	1.397735	4.057450	0.044895	1590.8113	1633.9753	1647.3121
	H	-1.012281	3.890921	-0.454513	1648.4962	1664.5696	1684.7653
	H	-3.028232	2.568793	-0.572452	2998.5249	3006.8921	3057.2518
	H	-0.508206	-1.555172	0.417820	3067.5429	3145.0094	3155.5888
	H	-3.280727	-2.466960	-0.803079	3157.6368	3159.5611	3161.0323
	H	-2.559691	-2.745068	0.778472	3169.6367	3176.9523	3179.1455
	H	-5.183384	1.223010	-0.692480	3186.4083	3204.7391	3227.7838
	H	-4.489976	-1.723190	1.911776			
	H	-5.139288	-2.787989	0.671140			
	C	1.592703	-0.391021	-0.194272			
	C	2.973605	-0.372133	0.174027	61.5776	68.7656	89.1101
	C	1.129370	-1.527036	-0.906175	97.8596	124.1437	170.6259
	C	0.770087	0.784351	0.052971	201.5465	242.7113	258.5418
	C	3.774084	-1.519804	-0.039510	290.1842	313.6863	346.3700
	C	3.554977	0.832681	0.669942	393.1114	417.2735	438.9533
	C	1.941364	-2.615278	-1.140237	454.4587	466.7266	488.0715
	C	1.449381	1.998053	0.328628	498.7294	523.6153	534.3683
	C	3.268873	-2.631235	-0.672903	540.9088	555.7426	598.9485
	C	2.833900	1.984909	0.679716	610.1381	626.1136	663.7311
	C	-0.677835	0.825596	-0.056367	675.0988	688.1840	697.6567
	C	0.766958	3.245278	0.211014	716.2255	754.3514	759.8619
	C	-1.287113	2.086885	-0.328137	780.7061	782.7588	789.6457
	C	-0.527562	3.288257	-0.200131	804.6892	817.7652	838.9143
	C	-2.659893	2.151324	-0.661019	854.3714	861.9650	881.7588
	C	-3.438004	1.016421	-0.656217	922.3340	930.5074	943.5773
	C	-1.561138	-0.300649	0.179776	957.3939	961.8735	963.8389
	C	-2.919702	-0.204131	-0.201925	967.7696	969.7161	978.4541
[i11]	C	-3.852647	-1.392495	-0.083034	994.8831	1046.0932	1063.2654
	C	-1.154184	-1.447819	0.934192	1071.7516	1115.6506	1153.3498
	C	-2.038401	-2.511284	1.203710	1169.0650	1175.3808	1179.9272
	C	-3.316581	-2.528401	0.728465	1182.8703	1194.4861	1201.3628
	H	0.122707	-1.530711	-1.297598	1206.3967	1231.8169	1241.0076
	H	4.811721	-1.491705	0.276615	1245.3722	1261.6730	1291.5445
	H	4.599016	0.827439	0.964300	1294.9750	1343.3477	1356.1091
	H	1.555353	-3.460053	-1.699568	1371.6883	1385.5589	1397.4768
	H	3.896522	-3.498447	-0.844126	1410.8031	1427.6795	1446.9375
	H	3.298886	2.924434	0.959247	1448.6890	1461.8540	1470.5073
	H	1.322728	4.158504	0.394740	1519.8608	1528.0215	1549.4078
	H	-1.023957	4.235842	-0.379728	1563.9244	1582.5301	1608.2515
	H	-3.092198	3.115138	-0.906903	1633.9187	1647.5407	1660.6848
	H	-4.485402	1.075868	-0.935505	2913.7769	2981.0136	3152.0201
	H	-4.817152	-1.061373	0.327493	3154.5640	3156.1663	3158.1428
	H	-4.102730	-1.752537	-1.097238	3159.7757	3169.2566	3173.5146
	H	-0.163628	-1.474303	1.361479	3175.3757	3176.0739	3178.7778
	H	-1.681340	-3.335881	1.812319	3184.7501	3217.5844	3226.9199
	H	-3.973982	-3.367031	0.929400			
	C	2.061343	-0.515061	-0.096935	42.1541	61.5713	80.4764
	C	3.445160	-0.341092	0.224868	103.6904	124.0656	164.3535
	C	1.675393	-1.791376	-0.582193	209.8928	228.8828	262.7026
	C	1.164844	0.628919	-0.012648	287.2977	318.8006	338.8615
	C	4.320323	-1.452150	0.201323	391.1733	407.7093	422.6976
[i7]	C	3.951592	0.965694	0.490886	446.1893	473.3271	487.0452
	C	2.557795	-2.850561	-0.630481	500.1022	519.9774	537.3973
	C	1.751444	1.915007	0.093930	550.9198	573.5804	593.2694
	C	3.886712	-2.694579	-0.199740	607.3671	635.9233	647.6405
	C	3.146049	2.053042	0.363518	663.9331	691.7298	713.6707
	C	-0.283229	0.548969	-0.029952	715.8284	754.4605	762.3306

	C	0.952913	3.089583	-0.063092	763.4713	781.6761	805.3775
	C	-1.047616	1.743635	-0.236108	808.7060	816.5094	839.3434
	C	-0.384349	3.007665	-0.284730	846.4024	881.8499	891.4394
	C	-2.447638	1.670189	-0.320450	904.7800	908.4891	942.3073
	C	-3.146780	0.477671	-0.133522	953.0943	954.8063	963.7839
	C	-1.020788	-0.634192	0.243445	966.8846	975.1235	980.7365
	C	-2.395464	-0.693601	0.201815	1002.8114	1022.2059	1067.0082
	C	-3.114556	-1.988480	0.535341	1072.6021	1125.2633	1162.2230
	C	-4.572746	0.408883	-0.226397	1171.2860	1172.8186	1182.4290
	C	-5.258664	-0.795277	0.009077	1188.5690	1198.4116	1205.7679
	C	-4.602338	-1.942190	0.364377	1223.5357	1230.6811	1243.7941
	H	0.681362	-1.931611	-0.978822	1257.0610	1289.8000	1305.4466
	H	5.357772	-1.296550	0.478622	1320.6272	1344.3833	1354.0761
	H	5.001896	1.077748	0.737708	1372.5395	1386.6154	1398.0658
	H	2.225716	-3.805018	-1.023526	1423.6947	1443.7987	1446.6507
	H	4.570974	-3.535032	-0.223009	1450.4148	1465.1837	1473.4725
	H	3.546587	3.053408	0.489415	1517.4835	1534.1840	1543.3468
	H	1.447943	4.054120	-0.023967	1561.9910	1586.7920	1625.9708
	H	-0.977617	3.901632	-0.444331	1631.5478	1646.9381	1663.2621
	H	-3.003845	2.583649	-0.508179	2952.6310	2976.7814	3154.0658
	H	-0.488611	-1.522997	0.552330	3155.3532	3157.2570	3159.2396
	H	-2.701044	-2.805967	-0.073278	3160.7993	3169.2224	3172.0154
	H	-2.879372	-2.277403	1.572435	3176.7726	3178.9677	3182.8012
	H	-5.122234	1.306488	-0.485754	3186.0736	3197.5094	3225.1270
	H	-6.339326	-0.810275	-0.090097			
	H	-5.156597	-2.856378	0.546474			
[4]helicenyl	C	-1.273969	-0.281465	0.050973			
	C	-2.448402	0.503591	-0.178006	79.0980	83.9753	128.1870
	C	-1.474592	-1.638515	0.414493	177.9813	211.4427	260.0142
	C	0.028722	0.364520	-0.000773	278.6239	325.1728	377.9785
	C	-3.720555	-0.114427	-0.186856	411.5753	438.3818	441.1265
	C	-2.337853	1.918854	-0.320386	477.4310	510.9803	525.5294
	C	-2.730084	-2.209316	0.432813	526.7403	552.4507	575.1484
	C	0.063747	1.779995	0.011437	593.2032	623.4733	672.6080
	C	-3.865463	-1.453409	0.093222	686.4891	703.7541	749.1795
	C	-1.136683	2.533814	-0.166146	757.1880	758.8876	776.4242
	C	1.298349	-0.338621	-0.067416	805.3191	824.4209	826.2772
	C	1.297945	2.472676	0.200413	851.4441	855.0845	877.5391
	C	2.514109	0.383060	0.168622	896.1644	952.4505	958.3356
	C	2.469545	1.799122	0.338041	966.7867	975.1529	982.8406
	C	3.763334	-0.284414	0.158659	1002.0446	1012.6423	1057.1376
	C	3.862465	-1.631340	-0.138003	1078.6439	1122.1064	1145.3288
	C	1.433077	-1.706085	-0.461674	1171.2432	1174.9236	1183.9830
	C	2.671335	-2.263196	-0.460788	1205.1101	1223.3171	1235.4796
	H	-0.635934	-2.234068	0.741140	1245.9869	1263.5857	1307.8496
	H	-4.590739	0.500608	-0.391349	1343.0963	1351.1362	1369.1997
	H	-3.238885	2.496481	-0.496887	1394.5929	1410.0419	1439.6083
	H	-2.840349	-3.245859	0.731017	1451.8378	1472.0577	1499.0507
	H	-4.847313	-1.912669	0.092076	1530.4077	1545.5977	1588.5720
	H	-1.061968	3.615493	-0.199122	1611.9531	1635.9618	1647.8789
	H	1.274918	3.555776	0.254148	1665.4207	3153.5571	3157.4577
	H	3.396815	2.331023	0.521542	3159.5646	3161.1358	3170.1760
	H	4.659181	0.291608	0.369653	3176.8116	3179.2223	3181.0244
	H	4.817602	-2.143189	-0.143273	3186.4303	3202.3191	3227.6458
	H	0.576509	-2.264272	-0.810689			
[i12]	C	2.047374	-1.219444	-0.300457	4.7337	10.2313	10.9347
	C	2.908689	-2.248367	0.189588	25.3461	32.8382	46.7352
	C	1.147947	-1.570127	-1.338191	67.0739	73.3060	91.5319
	C	2.222848	0.147402	0.175812	121.2898	172.7069	178.0729
	C	2.733262	-3.581469	-0.251722	228.1770	231.9721	246.1581
	C	4.000351	-1.909133	1.045447	278.7616	313.1916	319.2710
	C	1.025402	-2.868610	-1.782562	343.7574	399.5834	413.3331
	C	3.448462	0.447850	0.826612	419.6677	450.2333	470.1292
	C	1.799463	-3.895636	-1.211590	478.0634	496.9802	518.5379
	C	4.294331	-0.606589	1.292800	538.1107	545.7541	552.4314
	C	1.290713	1.235269	-0.043342	559.6726	567.3789	611.7140
	C	3.862148	1.799682	0.983135	626.3073	643.4824	650.4952
	C	1.800208	2.561197	-0.021161	673.5063	680.2990	691.4188
	C	3.105661	2.815833	0.482773	703.2950	717.3903	727.5107
	C	0.990973	3.652680	-0.465000	756.9544	767.2692	775.4715

	C	-0.306571	3.470252	-0.821631	782.3808	791.5710	810.1857
	C	-0.151665	1.089435	-0.186787	822.4485	839.0149	856.7963
	C	-0.934378	2.201359	-0.630816	860.1590	880.7933	884.8780
	C	-0.862026	-0.076543	0.229969	892.1123	931.6858	944.8645
	C	-2.209268	-0.100181	0.070419	956.2706	962.8736	966.1089
	C	-3.002113	0.911966	-0.451929	969.1217	976.3759	981.0508
	C	-2.337127	2.076552	-0.788872	999.1745	1009.2955	1048.0978
	H	0.554706	-0.799169	-1.807769	1063.1933	1082.6218	1091.9631
	H	3.379441	-4.350510	0.158568	1112.2884	1145.9897	1161.0689
	H	4.633128	-2.704007	1.425388	1173.3390	1178.7202	1184.3500
	H	0.333125	-3.095715	-2.585298	1201.2364	1215.1579	1228.9562
	H	1.684268	-4.918433	-1.551817	1233.4323	1244.5342	1268.4498
	H	5.181795	-0.337626	1.855777	1287.3929	1321.8502	1323.0475
	H	4.818477	1.998863	1.454517	1343.1439	1359.4951	1374.3827
	H	3.458770	3.840782	0.516260	1389.5037	1403.2926	1414.9798
	H	1.442825	4.637774	-0.510561	1442.7133	1446.3845	1450.6503
	H	-0.905716	4.300270	-1.180050	1467.3981	1497.0399	1513.7432
	H	-0.333083	-0.906775	0.677067	1536.2375	1549.3456	1582.7413
	H	-4.075433	0.812725	-0.565248	1610.0926	1621.4819	1648.3463
	H	-2.895471	2.932486	-1.155645	1653.4916	1660.5930	1668.2289
	C	-5.429048	-1.426779	2.100264	2201.8700	3134.8689	3143.4899
	C	-6.597344	-1.157841	1.508231	3153.5720	3157.2348	3158.9934
	C	-6.743076	-0.779198	0.144162	3159.8147	3161.7830	3171.0873
	C	-6.909738	-0.457236	-1.005087	3176.6923	3177.9280	3180.1113
	H	-5.391718	-1.708609	3.145592	3180.7581	3186.1448	3200.0095
	H	-4.489016	-1.369613	1.563774	3217.7612	3233.1486	3476.4033
	H	-7.519356	-1.223878	2.080748			
	H	-7.049601	-0.182515	-2.021679			
p7	C	1.588285	-0.544702	-0.499249			
	C	2.840640	-1.167607	-0.210020	47.6776	67.5148	68.7063
	C	0.734260	-1.203774	-1.416287	104.2938	113.8247	130.8369
	C	1.293987	0.765153	0.066848	180.0381	194.9433	246.0667
	C	3.129331	-2.446895	-0.740130	252.8712	258.8954	309.9693
	C	3.823678	-0.463051	0.550021	321.0205	369.0303	407.2560
	C	1.054950	-2.433294	-1.949598	421.7123	427.6531	436.2217
	C	2.382659	1.492757	0.613627	436.8204	474.8415	488.3495
	C	2.250236	-3.080010	-1.588111	512.3939	519.7071	530.2985
	C	3.620996	0.834590	0.894704	534.0044	546.0432	568.5214
	C	0.000000	1.422446	-0.000002	575.5197	619.9768	633.4147
	C	2.270898	2.894945	0.830728	645.4641	669.6508	688.7904
	C	0.000000	2.848382	-0.000004	705.2322	708.1572	751.2725
	C	1.151403	3.561787	0.436519	752.8798	756.8058	757.0350
	C	-1.151402	3.561786	-0.436528	768.2905	783.6581	805.3933
	C	-2.270897	2.894943	-0.830735	812.8710	817.8606	838.4626
	C	-1.293986	0.765153	-0.066850	841.6048	844.2637	859.4332
	C	-2.382659	1.492756	-0.613631	883.8664	884.6595	914.9288
	C	-1.588285	-0.544700	0.499251	929.7106	957.0747	963.3306
	C	-2.840640	-1.167605	0.210022	966.2949	969.3604	977.9604
	C	-3.823678	-0.463051	-0.550020	979.3353	996.8830	996.9297
	C	-3.620996	0.834589	-0.894707	998.4022	1052.6606	1062.1186
	C	-0.734260	-1.203770	1.416291	1068.1832	1113.7163	1137.7759
	C	-1.054951	-2.433288	1.949605	1164.4713	1165.8570	1177.8412
	C	-2.250237	-3.080005	1.588119	1178.5170	1184.6376	1185.4671
	C	-3.129331	-2.446893	0.740136	1205.7105	1211.0793	1231.4355
	H	-0.182533	-0.724281	-1.725847	1233.3410	1241.2520	1246.4316
	H	4.078050	-2.908846	-0.487143	1277.1503	1300.0189	1318.8713
	H	4.759427	-0.960254	0.782273	1357.1226	1359.0895	1369.9807
	H	0.380224	-2.900724	-2.657750	1382.0713	1384.7201	1393.1290
	H	2.488123	-4.055199	-1.997620	1421.0343	1448.9792	1449.7611
	H	4.401650	1.404433	1.387455	1465.9883	1471.3663	1506.6575
	H	3.123657	3.428621	1.236081	1516.6303	1537.5281	1548.0872
	H	1.102216	4.644317	0.483112	1557.2340	1586.3534	1613.5793
	H	-1.102215	4.644316	-0.483124	1641.6198	1648.7934	1648.8681
	H	-3.123656	3.428618	-1.236090	1660.3646	1661.1276	3156.1593
	H	-4.759427	-0.960255	-0.782271	3156.2803	3158.2366	3158.5004
	H	-4.401650	1.404430	-1.387459	3159.9732	3161.8142	3170.2632
	H	0.182532	-0.724276	1.725850	3170.3468	3175.8804	3176.3154
	H	-0.380225	-2.900716	2.657758	3178.5207	3180.3782	3185.2294
	H	-2.488124	-4.055193	1.997631	3185.5148	3219.5594	3219.7894
	H	-4.078051	-2.908845	0.487149			

p8	C	-1.832937	-0.998898	0.296910			
	C	-2.893943	-1.845577	-0.145389	43.9662	58.5227	69.2432
	C	-0.906833	-1.552054	1.215519	95.5722	118.8082	144.7491
	C	-1.828187	0.408562	-0.093855	171.2249	198.6926	231.1436
	C	-2.897694	-3.214572	0.212631	264.4361	278.5598	294.2637
	C	-3.995708	-1.285749	-0.863297	330.0936	353.7998	395.3912
	C	-0.955756	-2.879182	1.584437	408.4953	412.7214	443.1424
	C	-3.049930	0.937753	-0.594787	452.4389	478.2228	484.0898
	C	-1.939324	-3.732914	1.052514	499.8588	521.1562	534.0291
	C	-4.097499	0.058860	-1.016274	537.1135	554.1671	566.5979
	C	-0.717352	1.318785	0.068790	592.0134	614.4769	636.9766
	C	-3.249431	2.341530	-0.651788	641.7277	650.4817	693.2826
	C	-1.001327	2.704430	0.152795	704.5229	715.8527	751.1980
	C	-2.286001	3.194194	-0.197056	754.2833	759.8867	769.8406
	C	0.015894	3.629767	0.572268	778.3969	782.9217	797.8233
	C	1.287638	3.229062	0.803524	812.3772	814.8198	832.0212
	C	0.698747	0.935180	0.055147	842.6365	854.1828	860.4706
	C	1.691403	1.887779	0.493107	884.3920	899.7749	907.2767
	C	1.157689	-0.264405	-0.486991	926.1849	935.0868	951.6070
	C	2.516704	-0.615294	-0.506998	961.6142	968.4322	970.1431
	C	3.486247	0.291532	0.040809	977.5409	981.0529	995.0005
	C	3.038794	1.532706	0.511955	999.0252	1032.2676	1052.4463
	C	4.860585	-0.086115	0.038025	1073.6034	1097.3724	1144.3001
	C	4.297312	-2.183467	-1.035219	1163.3477	1167.1197	1176.5169
	C	5.254731	-1.289302	-0.482792	1182.0295	1183.9777	1193.8578
	C	2.968451	-1.854379	-1.049230	1210.3106	1213.6387	1230.1000
	H	-0.151321	-0.916218	1.653104	1242.6741	1252.9046	1286.8331
	H	-3.698515	-3.843873	-0.161577	1290.5821	1304.0846	1323.8607
	H	-4.783232	-1.946423	-1.209595	1355.5274	1360.1935	1365.6852
	H	-0.235269	-3.262218	2.298214	1374.3294	1401.6167	1417.9003
	H	-1.961371	-4.780307	1.331267	1420.5785	1444.9570	1448.6197
	H	-4.980139	0.498587	-1.468484	1461.3299	1473.3087	1507.0046
	H	-4.201059	2.718378	-1.010602	1509.5331	1536.5146	1543.9566
	H	-2.466442	4.262744	-0.151659	1575.2281	1591.1197	1616.2376
	H	-0.270599	4.666584	0.713254	1630.8063	1648.4986	1655.9334
	H	2.038545	3.930507	1.150790	1662.1246	1667.2697	3154.3064
	H	0.452106	-0.962611	-0.915439	3156.8163	3157.4054	3158.4012
	H	3.766454	2.259444	0.860204	3159.2342	3161.4645	3163.2820
	H	5.590862	0.600513	0.453520	3170.5998	3175.1565	3176.4001
	H	4.627851	-3.131004	-1.445517	3177.4882	3179.8280	3185.6742
	H	6.302941	-1.566487	-0.479911	3187.0506	3204.3135	3218.8564
	H	2.235552	-2.537007	-1.466102			
p6	C	0.653351	1.589881	0.455673	26.6117	49.6650	62.3632
	C	0.694225	2.964124	0.069542	77.7355	85.8940	97.7489
	C	-0.250871	1.236058	1.488500	120.2468	149.9432	159.0209
	C	1.617421	0.656568	-0.116512	195.0519	231.1975	246.7148
	C	-0.252746	3.872305	0.600353	262.9823	308.3415	316.7935
	C	1.747576	3.431131	-0.774583	341.4399	360.1521	412.4969
	C	-1.135157	2.148909	2.021593	418.0610	421.6084	442.8873
	C	2.757201	1.220157	-0.749598	465.2386	471.5740	485.4858
	C	-1.164775	3.474753	1.550188	496.3746	515.4367	540.8646
	C	2.771705	2.604447	-1.108404	543.3486	557.0344	574.9316
	C	1.548299	-0.786249	-0.011929	602.2982	617.8308	622.3446
	C	3.906072	0.420040	-0.997632	641.0551	670.0274	678.1529
	C	2.760003	-1.518166	-0.121477	689.2019	692.7632	721.6734
	C	3.937893	-0.883294	-0.602515	736.1476	758.2297	772.6837
	C	2.797022	-2.907811	0.215352	777.3964	794.1536	798.4457
	C	1.668146	-3.584003	0.553102	812.4392	830.9195	843.7892
	C	0.317523	-1.564315	0.102748	855.1405	860.8658	877.9652
	C	0.395206	-2.949970	0.444348	885.1241	891.7040	926.3439
	C	-0.949905	-1.050568	-0.244272	947.3942	960.6241	966.2107
	C	-2.116687	-1.801237	-0.149780	970.1345	977.7464	981.7570
	C	-2.020021	-3.145249	0.292105	989.9029	996.5419	999.7722
	C	-0.796696	-3.701100	0.569190	1036.5552	1055.6947	1087.2517
	C	-3.436122	-1.274603	-0.499179	1095.6729	1154.1764	1169.2656
	C	-3.762043	0.015358	-0.719048	1176.2591	1181.9295	1184.3435
	C	-5.067308	0.446674	-1.061100	1203.9502	1206.1437	1222.0271
	C	-6.167065	0.848035	-1.351168	1231.6710	1242.0782	1251.2799
	H	-0.236225	0.230878	1.883824	1287.5406	1294.5513	1312.1252
	H	-0.221646	4.904331	0.266937	1331.8278	1348.2736	1358.6047

	H	1.753367	4.473359	-1.074951	1368.0432	1374.1333	1400.3699
	H	-1.804666	1.842955	2.817368	1413.8674	1429.8024	1449.3874
	H	-1.876524	4.182765	1.958947	1464.7904	1471.3231	1509.3317
	H	3.626157	2.978907	-1.662021	1527.2938	1545.4827	1551.8057
	H	4.774126	0.884230	-1.452992	1583.7047	1617.9173	1640.4829
	H	4.842077	-1.473497	-0.704424	1648.0794	1652.7319	1659.7660
	H	3.757657	-3.411372	0.197023	1670.5952	2193.6163	3142.6841
	H	1.709047	-4.631411	0.831827	3151.3591	3157.8606	3158.3442
	H	-1.009570	-0.042627	-0.626766	3159.8764	3160.6127	3162.2801
	H	-2.922501	-3.740422	0.381068	3172.0991	3176.1784	3177.4260
	H	-0.723685	-4.745034	0.855358	3178.5746	3180.6185	3187.1867
	H	-4.230516	-2.012818	-0.568364	3217.1871	3218.9843	3477.6788
	H	-3.012345	0.796362	-0.626995			
	H	-7.138219	1.192141	-1.608824			
p5	C	0.866579	1.560552	0.459315			
	C	1.017361	2.926930	0.071711	25.8869	36.9318	48.5026
	C	-0.032163	1.285900	1.520208	69.5628	81.0340	88.5517
	C	1.725898	0.547385	-0.142621	121.2352	152.6198	158.6976
	C	0.174621	3.914692	0.634514	193.3159	221.1968	244.1453
	C	2.078937	3.300198	-0.807656	259.8867	289.0741	312.3580
	C	-0.812378	2.272547	2.082588	321.3945	355.1364	398.1160
	C	2.889038	1.008826	-0.814613	413.2536	421.8580	437.9048
	C	-0.737193	3.597138	1.614133	461.4426	469.3160	487.8971
	C	3.013722	2.386696	-1.175951	504.3394	527.5012	540.9513
	C	1.535510	-0.884139	-0.031122	543.7829	557.2923	575.1948
	C	3.955126	0.111279	-1.097952	603.2412	619.6926	639.4037
	C	2.675318	-1.718873	-0.176408	651.5560	670.4451	689.3687
	C	3.887326	-1.189276	-0.698911	693.5248	699.0725	727.5423
	C	2.602435	-3.105051	0.165686	742.5410	757.7745	776.3708
	C	1.430510	-3.680131	0.543619	792.4470	798.9879	808.1281
	C	0.247601	-1.553412	0.123947	814.1490	833.6290	846.6723
	C	0.214849	-2.938890	0.470865	863.2206	870.0560	884.5947
	C	-0.981966	-0.933025	-0.187309	931.1144	933.6117	939.5142
	C	-2.200190	-1.592810	-0.056998	947.5286	960.9733	967.5818
	C	-2.215663	-2.935969	0.405575	971.0304	978.4382	981.7028
	C	-1.032966	-3.585575	0.646062	999.1281	1001.4455	1006.4965
	C	-3.416650	-0.937578	-0.391237	1055.7293	1086.6537	1090.2941
	C	-4.453026	-0.377463	-0.674038	1106.6385	1154.3657	1168.3529
	C	-5.682900	0.247108	-0.997212	1175.3655	1180.8827	1184.5360
	C	-5.810880	1.509650	-1.427392	1205.2491	1216.1444	1231.8450
	H	-0.096855	0.281882	1.913455	1240.4976	1248.3199	1273.9942
	H	0.287726	4.940983	0.300971	1287.7426	1304.7245	1319.6193
	H	2.167392	4.338580	-1.108543	1333.4302	1357.0456	1366.7506
	H	-1.482271	2.024503	2.897899	1373.4799	1399.3499	1411.2993
	H	-1.368067	4.364953	2.047218	1418.8389	1446.6678	1450.3102
	H	3.878756	2.685108	-1.758605	1465.7571	1472.5529	1505.2293
	H	4.844651	0.498137	-1.583204	1526.8105	1542.2656	1550.7922
	H	4.733106	-1.855825	-0.827927	1581.2101	1617.4498	1643.5007
	H	3.514447	-3.690522	0.118557	1648.6450	1651.9742	1660.3143
	H	1.389843	-4.726268	0.827008	1664.7524	2295.1020	3128.5819
	H	-0.990948	0.081059	-0.557008	3145.8330	3157.3620	3158.8273
	H	-3.164675	-3.443152	0.528020	3159.7988	3161.8970	3164.3797
	H	-1.036883	-4.628619	0.944459	3171.8590	3176.9135	3178.1596
	H	-6.573302	-0.366613	-0.879177	3180.4297	3186.5629	3193.5139
	H	-4.950084	2.154427	-1.558314	3217.1079	3226.3816	3235.5609
	H	-6.785954	1.921116	-1.657643			
TS **[i12]-[i14]**	C	1.658595	1.304097	0.329499	-99.5335	9.5703	21.1817
	C	2.398590	2.442815	-0.113554	27.4561	56.5178	67.7300
	C	0.649703	1.527091	1.299819	75.3821	97.8485	121.8511
	C	2.056839	-0.025867	-0.116238	159.4042	179.9090	184.8910
	C	2.007621	3.739135	0.298405	227.7924	235.1465	247.4363
	C	3.583723	2.258318	-0.888697	279.5082	313.5575	344.5225
	C	0.316438	2.796545	1.719726	359.7155	399.8147	413.8999
	C	3.355005	-0.152489	-0.677118	420.0360	450.5638	469.8630
	C	0.975753	3.921129	1.189564	477.8146	495.7913	520.5907
	C	4.074328	1.009401	-1.098217	530.1052	542.3129	552.6778
	C	1.273602	-1.233294	0.053077	558.6100	569.1421	611.8657
	C	3.964400	-1.433052	-0.786658	628.5842	629.3833	652.2156
	C	1.964744	-2.473988	0.084818	674.6683	676.8402	690.6369
	C	3.324938	-2.543737	-0.325286	717.1748	718.4400	726.0682

	C	1.287489	-3.666429	0.488238	757.1387	770.8829	776.2334
	C	-0.044434	-3.666107	0.753812	778.2867	790.7064	810.2326
	C	-0.181478	-1.290876	0.095148	823.2487	839.5177	852.9400
	C	-0.828892	-2.499124	0.502548	859.8272	884.1923	885.5028
	C	-1.016921	-0.239535	-0.386963	894.2777	912.6536	938.8234
	C	-2.365665	-0.394356	-0.323257	945.1639	956.6959	962.9612
	C	-3.034800	-1.509630	0.164114	968.9964	976.2917	980.9810
	C	-2.243013	-2.568958	0.564229	985.1110	998.8768	1047.0333
	C	-3.918438	1.567440	-1.116966	1062.4715	1083.7919	1091.5400
	C	-5.114780	1.028487	-1.426929	1111.8893	1145.3565	1160.9348
	C	-6.173576	0.847700	-0.501942	1172.9262	1178.5187	1184.0434
	C	-7.093248	0.677209	0.260043	1201.4261	1215.4739	1229.0195
	H	0.140296	0.681073	1.737554	1233.2844	1244.4897	1271.7077
	H	2.566167	4.590507	-0.076459	1287.5289	1305.7273	1324.5513
	H	4.123414	3.133258	-1.234837	1345.2766	1359.6507	1374.3809
	H	-0.451924	2.925780	2.473595	1389.7507	1403.9951	1413.6653
	H	0.695921	4.918354	1.509609	1436.3302	1443.5354	1450.7278
	H	5.027794	0.866668	-1.595650	1467.1122	1498.8118	1513.4297
	H	4.969727	-1.497229	-1.188707	1536.8467	1549.1205	1583.4967
	H	3.820103	-3.508711	-0.320391	1604.5721	1612.9323	1621.2427
	H	1.868462	-4.578016	0.578614	1648.0907	1653.2162	1660.3113
	H	-0.544898	-4.570256	1.083258	2184.3285	3140.2614	3151.8006
	H	-0.573138	0.651762	-0.809308	3156.7419	3157.0639	3158.6739
	H	-4.116838	-1.559315	0.205555	3159.5162	3161.5229	3170.1941
	H	-2.701141	-3.491973	0.906737	3176.4953	3177.5894	3179.0786
	H	-3.168950	1.720343	-1.882185	3180.0218	3185.6156	3194.3252
	H	-3.717125	1.970992	-0.133294	3217.6430	3249.3469	3476.1790
	H	-5.297987	0.677893	-2.439265			
	H	-7.899022	0.537320	0.937870			
TS **[i12]-[i13]**	C	0.321081	-1.517726	0.647736	-189.3571	15.0460	19.7242
	C	1.090988	-2.682491	0.345602	30.7422	56.1041	65.8529
	C	0.771017	-0.706906	1.719459	74.4817	85.2165	108.0305
	C	-0.940892	-1.293110	-0.047879	122.9167	174.3345	183.2587
	C	2.326258	-2.898808	1.001711	228.5462	233.6156	246.2086
	C	0.564014	-3.668391	-0.543008	279.9677	312.7558	333.8629
	C	1.956740	-0.961812	2.373319	344.5873	399.8514	414.1597
	C	-1.504969	-2.405606	-0.726609	419.8936	450.5830	469.6726
	C	2.764629	-2.048882	1.991041	476.6530	493.4899	519.4376
	C	-0.709775	-3.561915	-1.001291	521.3472	541.4767	552.8732
	C	-1.702694	-0.060232	-0.022017	560.6054	569.2562	612.2262
	C	-2.876416	-2.393647	-1.102992	628.9859	650.9762	653.2649
	C	-3.100996	-0.139798	-0.260006	662.6891	676.2881	691.5334
	C	-3.669360	-1.332220	-0.787127	698.0015	719.1313	729.2362
	C	-3.940922	0.990123	-0.011602	756.7135	768.1806	774.5137
	C	-3.420309	2.188071	0.359631	782.0787	790.5584	809.2294
	C	-1.136835	1.274277	0.131563	822.8428	838.3214	854.3376
	C	-2.005480	2.383722	0.378817	859.0774	883.5919	893.2292
	C	0.240285	1.566962	-0.089785	898.8275	928.2796	944.1339
	C	0.676939	2.845692	0.061606	946.3307	948.0306	961.4193
	C	-0.120670	3.932653	0.401904	967.6778	974.9522	980.0486
	C	-1.473010	3.685730	0.544400	997.4824	1001.7521	1045.6000
	C	3.161144	3.174132	-0.296384	1060.5429	1083.5111	1090.8506
	C	3.547044	2.338914	-1.088123	1112.1070	1145.8706	1160.8376
	C	3.893036	1.356151	-2.044915	1173.0811	1178.3248	1184.0714
	C	4.188733	0.080433	-1.753187	1201.6728	1215.1141	1229.4892
	H	0.162875	0.123841	2.045790	1233.9095	1244.6585	1271.4043
	H	2.906064	-3.776314	0.734588	1287.7225	1316.2444	1324.9531
	H	1.168929	-4.537723	-0.777636	1345.2580	1359.4720	1373.9798
	H	2.262242	-0.323512	3.194500	1389.7723	1403.6358	1413.5125
	H	3.704435	-2.234845	2.498588	1442.0781	1443.8854	1450.6788
	H	-1.152750	-4.356808	-1.591959	1467.1485	1498.3420	1512.9758
	H	-3.288780	-3.269850	-1.591569	1536.6896	1548.6220	1582.8609
	H	-4.734964	-1.354880	-0.988187	1610.4356	1621.1885	1641.0399
	H	-5.012260	0.865159	-0.127188	1647.7458	1653.6694	1660.7286
	H	-4.067049	3.033249	0.569464	2122.2438	3133.6304	3147.1536
	H	0.921877	0.784860	-0.393962	3147.9746	3156.0823	3157.7074
	H	0.280487	4.933427	0.521470	3158.5625	3160.8892	3167.2123
	H	-2.157158	4.502184	0.755739	3170.7449	3175.9037	3177.0360
	H	3.076643	3.961482	0.412201	3179.5213	3185.2629	3202.1726
	H	3.914190	1.687960	-3.080357	3219.4532	3238.1578	3459.7009

	H	4.171846	-0.289394	-0.735073			
	H	4.445900	-0.620720	-2.537576			
TS **[i14]-p6**	C	0.722823	1.577115	0.472776			
	C	0.795536	2.951986	0.093290	-539.1572	25.5498	47.5163
	C	-0.174744	1.242360	1.517798	59.5891	71.4400	84.5658
	C	1.651327	0.621033	-0.120189	98.1990	119.8903	143.3446
	C	-0.117790	3.882738	0.643669	158.7332	193.3354	222.2697
	C	1.847959	3.394657	-0.764899	245.6846	253.0521	280.4496
	C	-1.025674	2.175880	2.069051	308.4916	331.1956	342.4515
	C	2.795794	1.156429	-0.768951	352.0001	363.0152	414.3903
	C	-1.025951	3.504698	1.605130	417.5211	421.5785	441.4407
	C	2.843194	2.541914	-1.120038	465.6687	471.1375	482.9344
	C	1.543846	-0.820146	-0.022576	496.6148	514.5628	540.8309
	C	3.917812	0.326166	-1.040410	543.1087	557.2165	574.6945
	C	2.732817	-1.584893	-0.156517	602.5239	617.9100	621.1142
	C	3.919917	-0.979908	-0.653373	641.2161	670.1238	677.5085
	C	2.736220	-2.977050	0.170740	689.2678	692.6609	721.6563
	C	1.594417	-3.623705	0.523091	736.2996	758.5558	772.3756
	C	0.294688	-1.564237	0.108742	777.5211	794.5887	798.7112
	C	0.338581	-2.953073	0.440036	812.6408	831.0059	843.2708
	C	-0.964853	-1.012125	-0.212291	854.2602	858.1056	866.9538
	C	-2.147935	-1.729940	-0.100823	885.4714	891.0823	924.5365
	C	-2.083999	-3.077262	0.334952	947.4300	960.8958	966.8432
	C	-0.872659	-3.670147	0.583842	970.6715	978.0993	982.0079
	C	-3.460864	-1.164822	-0.440368	988.2105	997.0871	1000.9152
	C	-3.723825	0.127529	-0.775376	1041.4490	1055.7893	1087.5275
	C	-4.993116	0.581130	-1.193132	1095.4983	1154.2127	1169.2601
	C	-6.067113	0.999585	-1.551289	1176.4166	1181.9307	1184.4674
	H	-0.181844	0.235103	1.908054	1198.0852	1205.9951	1220.5315
	H	-0.063233	4.915497	0.315555	1231.7470	1241.9335	1250.8683
	H	1.878044	4.438150	-1.059383	1287.2802	1294.4404	1310.0774
	H	-1.691515	1.883367	2.872838	1315.7175	1343.5504	1358.7295
	H	-1.711683	4.229544	2.028603	1368.9194	1374.4680	1400.2182
	H	3.698774	2.895919	-1.685240	1413.7318	1429.0679	1449.4092
	H	4.790919	0.768963	-1.507260	1464.7286	1471.5142	1509.6997
	H	4.805552	-1.594280	-0.773596	1526.3227	1545.7688	1550.9369
	H	3.681780	-3.507346	0.132916	1584.2133	1607.3113	1621.4453
	H	1.610347	-4.673662	0.794583	1647.7738	1651.2380	1652.8355
	H	-1.000552	-0.000329	-0.586738	1660.4430	2180.5073	3148.4134
	H	-3.002303	-3.643892	0.444088	3157.8947	3158.2180	3159.2355
	H	-0.824848	-4.716922	0.864722	3160.4307	3161.2472	3162.4691
	H	-4.221552	-1.141941	1.518821	3172.7595	3176.9781	3177.7613
	H	-4.264677	-1.885177	-0.557194	3179.0712	3180.7550	3187.4151
	H	-2.946652	0.882280	-0.700053	3217.1813	3221.4432	3476.5979
	H	-7.014995	1.359240	-1.868015			
TS **[i14]-[i16]**	C	-1.447666	-0.637743	-0.637729	-1692.2185	28.9924	50.4097
	C	-2.827722	-0.795793	-0.307400	57.4317	75.6100	85.5581
	C	-1.133129	0.238332	-1.705986	124.7079	130.5515	150.8512
	C	-0.456913	-1.478855	0.018089	196.6326	212.7793	233.6868
	C	-3.797187	0.026283	-0.929132	246.3572	267.8326	300.3708
	C	-3.227904	-1.849988	0.569593	316.8004	367.9337	379.5467
	C	-2.102857	0.992316	-2.332105	416.1375	419.4595	424.0605
	C	-0.931428	-2.637887	0.684692	441.2065	471.6773	476.9401
	C	-3.445669	0.916729	-1.917453	486.5604	511.9453	528.6363
	C	-2.322663	-2.772626	0.987067	537.1622	541.0674	553.8014
	C	0.972182	-1.265997	-0.031581	574.9314	583.2941	616.1366
	C	-0.029071	-3.683377	1.026130	617.2777	643.5359	658.4074
	C	1.824756	-2.380131	0.184316	663.9168	687.3230	697.8685
	C	1.290243	-3.594680	0.697089	720.2742	725.6609	755.5727
	C	3.228087	-2.273233	-0.067001	759.9481	777.3138	783.4713
	C	3.796842	-1.090667	-0.420891	807.2240	810.4220	831.7650
	C	1.610749	0.031851	-0.181069	839.0388	847.1132	856.0496
	C	3.022399	0.108571	-0.427544	861.0768	881.1984	882.8858
	C	0.988369	1.270913	0.032442	939.3573	948.6150	957.0663
	C	1.593999	2.497367	-0.058049	962.1531	966.9837	974.5209
	C	2.957029	2.551639	-0.419419	979.9362	994.3726	996.6950
	C	3.647297	1.371935	-0.585923	1017.7611	1056.4698	1074.1360
	C	0.696286	3.658381	0.318388	1086.1096	1103.9341	1147.4094
	C	-1.246118	3.255144	1.917842	1166.2108	1173.3153	1178.5159
	C	-1.714563	3.423132	3.017903	1183.9466	1185.3180	1201.6878

	C	-0.676776	3.023784	0.632379	1208.0986	1220.7441	1232.0945	
	H	-0.115148	0.295371	-2.061897	1240.9955	1247.4191	1281.9672	
	H	-4.836002	-0.088363	-0.637750	1288.4151	1301.6411	1336.0979	
	H	-4.277128	-1.944326	0.828030	1347.9589	1361.1985	1361.8462	
	H	-1.828323	1.636426	-3.160160	1377.2626	1390.0468	1407.8364	
	H	-4.200797	1.526655	-2.400275	1412.8626	1446.3041	1452.9526	
	H	-2.638363	-3.632828	1.567859	1468.0361	1482.8665	1505.2858	
	H	-0.422968	-4.573676	1.504423	1519.3517	1541.3614	1546.1210	
	H	1.965056	-4.424242	0.878347	1576.5088	1616.3381	1640.3230	
	H	3.834256	-3.167078	0.034978	1646.7533	1651.0137	1659.7077	
	H	4.859600	-1.026645	-0.629562	1671.3732	2165.8422	3030.7681	
	H	3.463999	3.505836	-0.524400	3065.7991	3097.0873	3152.1779	
	H	4.709318	1.391514	-0.807069	3156.7375	3157.3584	3159.0660	
	H	0.615205	4.392473	-0.490138	3160.9452	3168.2960	3171.3714	
	H	1.089850	4.187523	1.190673	3175.7038	3177.0187	3179.4956	
	H	-2.130572	3.574489	3.983252	3184.4782	3219.5335	3476.4468	
	H	-0.295739	1.803963	0.511698				
	H	-1.403675	3.110502	-0.175901				
	C	1.818884	1.168543	0.273267				
	C	2.691120	2.179866	-0.232949	-1655.2200		26.1341	52.5355
	C	0.923515	1.545723	1.305519	60.2141	74.9373	94.4405	
	C	1.979315	-0.208315	-0.179916	110.9155	140.5122	147.5169	
	C	2.529920	3.522043	0.186460	191.6563	216.8240	234.9786	
	C	3.779313	1.814746	-1.082784	257.2770	278.3148	295.2046	
	C	0.815847	2.852431	1.729649	317.0400	342.7180	378.6877	
	C	3.203097	-0.532698	-0.822916	407.0904	411.5354	422.4967	
	C	1.600381	3.862080	1.141530	446.2938	450.6529	482.2419	
	C	4.059653	0.505048	-1.307067	488.5747	506.8051	532.3491	
	C	1.035411	-1.281807	0.058564	540.5209	543.6843	554.0202	
	C	3.603883	-1.891064	-0.953463	582.2859	594.6529	613.4715	
	C	1.535045	-2.611005	0.068130	623.1146	641.6906	658.0980	
	C	2.837579	-2.888805	-0.431333	667.6593	687.1230	696.7768	
	C	0.718484	-3.683869	0.542961	721.4312	738.0753	756.7234	
	C	-0.574448	-3.479491	0.905483	759.6935	775.7834	790.3506	
	C	-0.407682	-1.115402	0.196637	796.6444	813.0026	825.4090	
	C	-1.190562	-2.210928	0.683710	834.3530	844.4603	853.6207	
	C	-1.089884	0.044121	-0.256718	877.6225	879.0967	884.1753	
	C	-2.458784	0.159523	-0.133468	913.7976	941.5871	953.4007	
	C	-3.168662	-0.893905	0.452270	960.7104	967.9827	971.5998	
TS **[i14]-[i15]**	C	-2.596854	-2.063542	0.849061	975.7373	980.4103	997.7721	
	C	-3.350060	1.297832	-0.591208	1024.4874	1053.5325	1073.9717	
	C	-5.881408	1.052444	-0.840589	1080.1755	1095.6449	1154.0398	
	C	-6.846928	1.067067	-1.564974	1169.2836	1177.0568	1181.8231	
	C	-4.740050	0.993084	0.011483	1187.2279	1188.0568	1197.4121	
	H	0.323546	0.787823	1.787813	1218.4750	1226.7789	1231.1748	
	H	3.184363	4.277221	-0.236315	1244.1957	1259.1025	1278.7819	
	H	4.420491	2.596233	-1.476165	1286.9056	1298.2792	1324.3810	
	H	0.129984	3.099477	2.532223	1354.3729	1361.5987	1365.5384	
	H	1.497530	4.891313	1.466028	1374.8420	1393.3403	1400.0091	
	H	4.944590	0.217204	-1.864696	1412.7483	1442.5476	1450.7158	
	H	4.558021	-2.109013	-1.420901	1468.0645	1481.6295	1505.1832	
	H	3.180934	-3.917579	-0.442593	1511.2456	1542.8091	1546.9722	
	H	1.161465	-4.671798	0.611268	1584.2403	1617.2604	1630.9708	
	H	-1.179241	-4.292873	1.291576	1648.1889	1652.0570	1659.8803	
	H	-0.527764	0.842373	-0.722456	1662.4621	2168.1979	3040.1269	
	H	-3.172891	-2.894324	1.243833	3068.2480	3083.5981	3156.7588	
	H	-3.411200	1.323278	-1.682818	3157.1940	3158.8487	3159.5124	
	H	-2.978176	2.273838	-0.266773	3161.5798	3169.4356	3176.4705	
	H	-7.696409	1.088752	-2.202210	3177.4425	3179.9238	3185.2711	
	H	-4.908393	1.478017	0.975293	3197.3773	3216.8267	3475.5655	
	H	-4.483601	-0.212259	0.362858				
	C	-1.183578	-1.472942	0.438658	-599.3401	27.7882	30.2147	
	C	-1.534441	-2.793421	0.022360	57.6711	67.2817	76.0362	
	C	-0.302136	-1.356801	1.542449	96.6985	112.0175	121.6982	
	C	-1.839838	-0.328915	-0.183993	142.2646	166.0321	189.6268	
TS **[i13]-p5**	C	-0.888820	-3.909489	0.605637	231.2483	244.5477	258.4281	
	C	-2.600429	-2.982101	-0.909123	297.8757	312.6084	328.6047	
	C	0.282367	-2.461635	2.122341	343.9391	400.4962	408.6922	
	C	-3.029444	-0.589959	-0.914674	422.1851	427.7096	457.6456	
	C	0.016173	-3.752338	1.629472	464.3899	473.6567	489.0953	

	C	-3.357648	-1.926205	-1.303674	499.7768	516.7890	540.9993
	C	-1.426948	1.052018	-0.040231	544.7508	557.4807	590.7034
	C	-3.922605	0.470773	-1.230416	603.9858	619.9789	637.3832
	C	-2.409382	2.061420	-0.222242	653.0087	670.0846	689.4427
	C	-3.665024	1.739570	-0.807225	693.4898	699.8088	727.9222
	C	-2.130084	3.414169	0.146199	742.9174	758.0875	776.6644
	C	-0.900031	3.788559	0.586293	792.8505	799.2622	809.2547
	C	-0.057490	1.502914	0.184082	814.5687	833.8229	846.5826
	C	0.182266	2.860862	0.555504	863.4233	870.3938	884.9556
	C	1.070306	0.694330	-0.082141	933.5533	934.8751	937.5291
	C	2.368365	1.149327	0.113551	947.6191	961.2698	968.0191
	C	2.580524	2.462728	0.605374	971.4715	978.8950	982.0685
	C	1.508373	3.294097	0.800423	999.9697	1000.4257	1001.9431
	C	3.475973	0.300617	-0.205637	1055.8500	1086.9815	1090.2385
	C	4.298790	-0.425596	-0.739193	1105.3968	1154.4370	1168.4203
	C	5.280137	-1.296667	-1.257459	1175.5629	1181.0644	1184.7351
	C	6.538143	-0.937148	-1.558356	1205.0978	1216.0266	1231.8664
	H	-0.094697	-0.380278	1.955065	1240.3684	1247.9452	1269.4642
	H	-1.150508	-4.900960	0.250918	1287.6337	1303.4072	1315.5501
	H	-2.841115	-3.989787	-1.230438	1334.4677	1356.9625	1366.2015
	H	0.945344	-2.332190	2.970064	1373.5633	1399.2325	1410.9280
	H	0.494262	-4.615963	2.077468	1418.1688	1445.2925	1449.8688
	H	-4.231479	-2.075603	-1.928897	1465.6609	1471.4430	1506.2686
	H	-4.839235	0.237231	-1.761093	1526.6444	1543.3925	1550.7459
	H	-4.385509	2.535180	-0.962688	1581.6985	1617.6103	1638.2470
	H	-2.932545	4.139928	0.068027	1648.2011	1650.2475	1652.6308
	H	-0.704684	4.811458	0.889296	1660.4216	2222.4119	3131.1882
	H	0.933338	-0.303915	-0.469101	3147.3865	3157.3960	3159.0286
	H	3.591596	2.804176	0.788062	3159.8916	3162.0518	3165.5632
	H	1.666647	4.318980	1.118864	3172.3685	3176.9897	3178.3663
	H	4.329930	0.310940	1.627648	3180.5375	3186.7558	3196.4641
	H	4.968092	-2.326915	-1.413293	3217.2846	3227.0391	3238.1904
	H	6.886652	0.078840	-1.417516			
	H	7.242796	-1.660121	-1.950266			
TS **[i16]-[i17]**	C	-1.571091	-0.415442	0.520257	-435.0030	46.2554	56.2006
	C	-2.833615	-0.992662	0.185494	66.1996	82.6780	102.2140
	C	-0.769009	-1.112665	1.456323	110.2426	143.0397	162.9964
	C	-1.228083	0.901540	-0.000656	202.9212	219.9274	241.0264
	C	-3.171551	-2.277612	0.671431	261.1287	302.2182	312.2198
	C	-3.782169	-0.234465	-0.566410	329.8725	356.5873	368.9893
	C	-1.141093	-2.344074	1.951558	411.0753	419.0159	428.0291
	C	-2.286016	1.680509	-0.541524	450.2861	472.3299	478.1204
	C	-2.337304	-2.953688	1.530913	487.6452	508.3625	532.0248
	C	-3.539247	1.069403	-0.859670	540.4222	551.6483	569.2784
	C	0.083432	1.507103	0.078470	588.1791	615.6706	636.6065
	C	-2.117959	3.079758	-0.732035	655.7577	667.5823	672.5187
	C	0.166266	2.924925	0.044918	686.0816	705.4852	725.0425
	C	-0.960257	3.693555	-0.357869	745.6588	754.2864	758.5070
	C	1.386430	3.584181	0.392489	776.0993	783.9338	798.4241
	C	2.508716	2.879691	0.694565	807.5163	817.4751	833.9596
	C	1.342701	0.775548	0.124339	839.8725	855.4589	864.2633
	C	2.536591	1.463785	0.519727	869.6005	880.6903	931.6007
	C	1.517381	-0.549820	-0.306158	941.6312	953.5199	960.1576
	C	2.685609	-1.265355	-0.240631	964.3464	973.0154	978.7960
	C	3.810907	-0.595559	0.310738	992.7147	993.6349	1008.8205
	C	3.741236	0.734086	0.650960	1026.7659	1057.3932	1081.5196
	C	2.891725	-2.666727	-0.799607	1101.2362	1148.9703	1166.2156
	C	0.645441	-2.648398	-1.764835	1170.6836	1179.0768	1180.6707
	C	0.169946	-1.530040	-1.906664	1184.3856	1200.5857	1207.2793
	C	1.613337	-3.491413	-1.064146	1214.8364	1229.9461	1237.7435
	H	0.140905	-0.658802	1.817457	1242.9839	1257.0897	1287.9213
	H	-4.123758	-2.707238	0.378131	1320.2196	1337.6802	1347.6999
	H	-4.727312	-0.696443	-0.831155	1360.8956	1368.6701	1374.1354
	H	-0.510751	-2.838534	2.682462	1388.0539	1394.6403	1409.4132
	H	-2.614569	-3.930915	1.909906	1446.2075	1452.3528	1465.6317
	H	-4.296315	1.677741	-1.343224	1472.1537	1478.5209	1493.7792
	H	-2.951087	3.654965	-1.121385	1518.0032	1534.7343	1546.7904
	H	-0.861191	4.772430	-0.410523	1572.4746	1613.0070	1640.5612
	H	1.389356	4.668515	0.425228	1648.1959	1649.6476	1659.7923
	H	3.418188	3.386307	1.000340	2041.6093	3010.2538	3024.6911

	H	4.749983	-1.132438	0.411737	3049.3493	3060.6693	3143.3101
	H	4.627309	1.253925	0.999576	3155.6084	3156.1032	3157.8829
	H	3.537716	-3.230726	-0.118625	3160.1073	3167.1823	3170.0410
	H	3.445722	-2.574661	-1.741845	3174.8354	3175.9574	3178.8122
	H	-0.434228	-0.727401	-2.261695	3183.5907	3228.2895	3428.0583
	H	1.167166	-3.820745	-0.119180			
	H	1.868901	-4.392948	-1.629073			
TS **[i15]-[i18]**	C	-1.697396	-1.102844	0.297213			
	C	-2.673017	-2.063262	-0.110233	-366.8353	36.8712	49.9185
	C	-0.674096	-1.552457	1.169172	67.5202	78.9808	103.4421
	C	-1.871126	0.296870	-0.073636	122.6265	140.8533	165.6135
	C	-2.503085	-3.426552	0.230273	203.9066	213.7377	251.9188
	C	-3.860332	-1.627252	-0.773300	269.2020	291.3032	320.8199
	C	-0.555615	-2.878725	1.524445	343.7019	351.9093	378.0636
	C	-3.163747	0.687590	-0.512767	407.9630	416.7281	421.2364
	C	-1.456708	-3.836731	1.023260	445.8385	469.9097	482.8199
	C	-4.120821	-0.300674	-0.902921	495.0939	504.7419	530.7147
	C	-0.862155	1.328316	0.062431	541.7384	554.0356	559.4362
	C	-3.528465	2.062374	-0.528675	611.5673	621.2849	635.0547
	C	-1.305011	2.671268	0.199407	656.6299	660.4713	679.3394
	C	-2.655978	3.011192	-0.088448	691.1854	707.0508	725.7381
	C	-0.386780	3.695638	0.586200	739.6122	746.3209	757.7661
	C	0.938023	3.434950	0.741522	775.2176	789.2161	797.1932
	C	0.577266	1.112656	-0.019075	811.7493	816.2252	834.5061
	C	1.462358	2.157786	0.382730	850.9461	854.8663	865.3938
	C	1.149487	-0.044840	-0.607832	871.4446	884.0352	916.9674
	C	2.517423	-0.234633	-0.715224	923.9892	944.8495	957.3606
	C	3.337541	0.779327	-0.198025	962.5911	967.4708	974.0331
	C	2.868421	1.939508	0.331565	979.8474	995.6388	998.2870
	C	3.092362	-1.453991	-1.405267	1029.3597	1053.8254	1080.7710
	C	5.141774	-1.254498	-0.075288	1095.6282	1155.3884	1169.0903
	C	5.481642	-0.116386	0.206080	1176.6234	1183.3206	1189.2409
	C	4.149388	-2.213081	-0.553125	1193.4688	1197.2177	1211.7714
	H	0.019747	-0.835544	1.583415	1222.3313	1230.0509	1235.2071
	H	-3.241564	-4.141441	-0.117589	1245.3126	1280.6665	1286.9843
	H	-4.582054	-2.370101	-1.095715	1318.9997	1325.1921	1349.5385
	H	0.230371	-3.181100	2.207441	1358.0510	1367.4196	1375.5853
	H	-1.347378	-4.881457	1.291415	1391.6870	1399.8780	1411.4621
	H	-5.067121	0.038965	-1.310563	1439.8747	1449.8184	1467.6874
	H	-4.532600	2.330513	-0.838840	1476.2875	1482.3545	1495.6333
	H	-2.958293	4.049792	-0.007990	1511.0887	1539.5455	1546.1102
	H	-0.776778	4.693635	0.756564	1580.1023	1609.8606	1626.2706
	H	1.624437	4.211714	1.061106	1647.9921	1651.0332	1659.6006
	H	0.493662	-0.801135	-1.018386	2066.6298	3025.4156	3028.2429
	H	3.532111	2.724846	0.682236	3061.2784	3080.7125	3141.7438
	H	3.579206	-1.142911	-2.335765	3156.2776	3156.9892	3158.5148
	H	2.288036	-2.143828	-1.672412	3160.7014	3168.5915	3175.5068
	H	6.054454	0.722813	0.525425	3176.4960	3179.2298	3184.5267
	H	4.605942	-3.003883	-1.156137	3192.5554	3216.7238	3435.2484
	H	3.669722	-2.700186	0.302881			
TS **[i17]-[i19]**	C	-1.570244	-0.503393	0.483153	-1519.9364	50.0908	63.4318
	C	-2.821911	-1.117543	0.179144	69.3598	101.2460	108.0727
	C	-0.727532	-1.170034	1.405680	123.5587	147.2747	183.1096
	C	-1.273282	0.815953	-0.058859	228.1725	244.3324	251.1858
	C	-3.115120	-2.404380	0.687990	289.0916	313.7385	328.0982
	C	-3.802165	-0.395017	-0.567898	368.4357	406.5659	415.6282
	C	-1.054500	-2.405583	1.921914	423.4930	436.0561	461.1229
	C	-2.360120	1.560933	-0.585670	475.9511	489.6166	496.5382
	C	-2.245648	-3.048728	1.536790	517.6126	524.0567	539.6662
	C	-3.599757	0.911024	-0.880452	549.9420	567.6368	602.0319
	C	0.022623	1.461499	0.010010	607.0326	622.9443	655.7108
	C	-2.237007	2.965300	-0.773774	665.1860	671.7016	692.8763
	C	0.042651	2.884974	0.029501	721.9149	730.6867	739.5050
	C	-1.105487	3.616179	-0.380073	750.4592	756.0489	775.0074
	C	1.214142	3.576011	0.463758	777.7143	790.1036	804.2434
	C	2.330799	2.893033	0.829673	809.1136	838.6738	840.2723
	C	1.307487	0.784263	0.051209	843.2616	857.9481	872.2221
	C	2.423404	1.488012	0.591897	882.5647	925.1906	933.5361
	C	1.552584	-0.514849	-0.534545	946.7939	957.3416	964.0347
	C	2.788156	-1.159244	-0.296495	966.4279	972.6980	978.4716

	C	3.797352	-0.507781	0.424156	984.3500	992.1846	1043.9129
	C	3.639975	0.803674	0.818722	1057.6135	1081.0610	1101.6607
	C	3.087227	-2.492675	-0.960071	1132.0337	1165.5774	1169.6988
	C	0.660810	-2.545953	-1.696391	1177.7856	1183.9170	1187.0822
	C	0.653211	-1.140269	-1.463778	1192.3347	1204.7967	1217.9890
	C	1.820830	-3.235035	-1.311575	1224.7046	1232.9521	1240.0709
	H	0.183797	-0.690954	1.733032	1244.0410	1256.6926	1284.1222
	H	-4.060270	-2.863649	0.418089	1290.0983	1310.2362	1349.3634
	H	-4.737266	-0.886504	-0.813969	1354.9664	1359.7140	1368.8227
	H	-0.393591	-2.877086	2.640976	1375.6596	1389.0904	1403.0135
	H	-2.488741	-4.028742	1.931396	1406.7359	1434.7490	1442.3683
	H	-4.380298	1.492354	-1.359759	1450.7447	1456.7921	1465.9735
	H	-3.087616	3.514950	-1.162070	1502.9294	1519.5373	1541.0085
	H	-1.047616	4.698878	-0.410302	1545.6845	1571.7558	1596.3517
	H	1.177010	4.657946	0.532445	1620.3564	1647.8399	1648.2025
	H	3.195460	3.411172	1.230070	1658.6469	2118.8476	2956.6375
	H	4.739625	-1.017275	0.599064	3046.8645	3120.2505	3154.3907
	H	4.460306	1.338551	1.284930	3157.2169	3158.6518	3159.4256
	H	3.742307	-3.097859	-0.325608	3161.3778	3167.3945	3174.2536
	H	3.647257	-2.311022	-1.891781	3176.3223	3176.7369	3178.2432
	H	-0.075016	-0.527591	-1.980646	3179.9509	3184.4276	3214.4138
	H	0.695131	-3.214288	-0.597960			
	H	1.858637	-4.321098	-1.372011			
TS **[i18]-[i20]**	C	-1.783916	-1.035462	0.296905			
	C	-2.817282	-1.924129	-0.131812	-1521.2506	42.6956	58.0571
	C	-0.813276	-1.556082	1.189618	68.7182	90.9441	116.3883
	C	-1.847911	0.370441	-0.079968	128.7121	152.9432	190.8712
	C	-2.752320	-3.295522	0.211653	210.1525	234.3569	274.3371
	C	-3.954560	-1.405176	-0.821931	285.2421	311.4835	329.5944
	C	-0.796569	-2.887262	1.545217	360.9042	383.7684	412.6974
	C	-3.096334	0.853100	-0.552964	423.1087	442.4422	453.6249
	C	-1.753684	-3.778536	1.025021	476.5516	495.1263	503.9725
	C	-4.114496	-0.063680	-0.962034	512.9793	523.5681	542.2436
	C	-0.768805	1.326805	0.078648	548.9809	557.1664	599.7178
	C	-3.357233	2.251070	-0.582373	613.1770	622.5776	642.0092
	C	-1.114351	2.702312	0.197212	672.8470	688.7167	698.0053
	C	-2.427903	3.137414	-0.125331	722.3073	727.9585	742.7443
	C	-0.129990	3.660310	0.594042	757.7634	760.5964	776.3594
	C	1.168704	3.305622	0.772097	782.9821	795.9562	801.3246
	C	0.645417	1.007057	0.029100	814.6656	826.7789	832.4992
	C	1.605349	1.987103	0.434422	845.0299	856.0511	884.4070
	C	1.151858	-0.194706	-0.542823	890.6109	913.2108	921.9007
	C	2.491335	-0.480109	-0.599246	936.9639	950.7735	961.4650
	C	3.447731	0.440951	-0.050745	968.2744	971.7818	975.7915
	C	2.974485	1.665977	0.425740	981.0634	997.9717	1048.4780
	C	3.019291	-1.707392	-1.320816	1056.3551	1077.9351	1098.6212
	C	5.261141	-1.275880	-0.174353	1145.4120	1168.6341	1170.7927
	C	4.833211	0.084433	-0.059983	1178.4562	1184.0164	1191.3283
	C	4.312337	-2.179512	-0.690395	1193.4203	1207.6731	1219.3627
	H	-0.080301	-0.889829	1.620717	1228.1061	1233.2843	1244.6585
	H	-3.532472	-3.956382	-0.151544	1249.4067	1286.8174	1289.9565
	H	-4.721064	-2.094743	-1.158876	1300.2692	1305.7420	1336.9496
	H	-0.047529	-3.245214	2.242577	1350.5375	1360.5964	1370.8538
	H	-1.724396	-4.828191	1.294371	1380.4036	1392.7167	1412.0501
	H	-5.023791	0.342197	-1.392490	1427.5991	1433.0397	1449.2169
	H	-4.331016	2.590925	-0.917867	1455.0135	1464.6775	1470.8867
	H	-2.655694	4.195724	-0.058613	1503.1611	1514.7013	1533.7446
	H	-0.449370	4.685014	0.751301	1549.1779	1580.0716	1613.7643
	H	1.904842	4.032219	1.098437	1618.1022	1647.6165	1649.5127
	H	0.455022	-0.894350	-0.984004	1658.7655	2127.2064	2967.5921
	H	3.686045	2.404175	0.782924	3069.6895	3119.2461	3145.8924
	H	3.231474	-1.443006	-2.368750	3156.7087	3157.3423	3159.3317
	H	2.269704	-2.502109	-1.343510	3160.0805	3162.4697	3169.8507
	H	5.575835	0.861486	0.094851	3177.6736	3177.9560	3180.4076
	H	4.547736	-3.241284	-0.736229	3185.8496	3198.8344	3216.6126
	H	4.601613	-2.071520	0.597295			
TS **[i19]-p7**	C	1.572875	-0.609941	-0.498831	-623.7860	46.8322	66.8532
	C	2.791171	-1.296166	-0.207085	68.1359	102.8989	113.1261
	C	0.682751	-1.230351	-1.408466	129.8944	175.1962	192.3748
	C	1.349643	0.717634	0.058845	244.1086	246.7485	256.7996

	C	3.009807	-2.593546	-0.726591	279.5988	304.8027	322.3368
	C	3.812489	-0.638666	0.544538	345.7633	370.6656	407.9128
	C	0.934981	-2.480649	-1.930454	424.5212	431.2111	436.2572
	C	2.476578	1.390416	0.598701	453.4700	475.6359	489.5037
	C	2.095139	-3.186694	-1.565825	517.2626	523.4426	531.4742
	C	3.679769	0.670237	0.880389	531.9578	545.6008	568.4212
	C	0.091520	1.441421	-0.006336	578.6197	621.8181	634.0915
	C	2.438906	2.797445	0.809008	642.6622	669.8930	689.0278
	C	0.164591	2.865430	-0.009577	703.4587	707.6965	750.8421
	C	1.353508	3.520065	0.417661	752.6130	757.1422	759.1774
	C	-0.951574	3.637015	-0.439853	772.1545	785.9158	808.7951
	C	-2.107529	3.029797	-0.823525	813.8065	820.3117	839.2076
	C	-1.235237	0.852174	-0.066058	842.2761	843.9029	860.2230
	C	-2.290084	1.635044	-0.603755	884.8814	899.4712	915.1334
	C	-1.593180	-0.441491	0.499178	929.4717	957.6977	964.9454
	C	-2.873684	-0.999546	0.212674	968.7656	973.9185	979.4390
	C	-3.826061	-0.247234	-0.531471	982.1765	996.2496	999.6321
	C	-3.561846	1.042196	-0.872783	1001.3648	1053.4941	1062.8996
	C	-3.214334	-2.287212	0.721832	1066.2861	1112.8043	1133.9335
	C	-0.775407	-1.133808	1.425961	1160.9964	1165.5197	1176.6610
	C	-1.165482	-2.334921	1.987178	1178.3553	1184.7613	1185.7208
	C	-2.382622	-2.926777	1.633748	1204.8241	1211.3276	1227.5914
	H	-0.208002	-0.706085	-1.721223	1232.7248	1241.0851	1246.3280
	H	3.933351	-3.103121	-0.471915	1274.9796	1297.5850	1318.3607
	H	4.721491	-1.182847	0.777687	1350.9964	1358.2630	1370.1609
	H	0.231974	-2.918693	-2.629446	1379.6056	1384.7538	1391.3627
	H	2.278512	-4.177392	-1.965922	1419.2643	1445.0296	1449.1766
	H	4.490953	1.201678	1.366638	1460.7242	1468.8592	1505.9469
	H	3.320246	3.287827	1.207843	1515.2382	1536.3309	1547.3271
	H	1.360765	4.603826	0.460002	1554.4856	1582.1862	1610.0621
	H	-0.845751	4.715323	-0.489793	1623.4647	1638.6027	1648.6779
	H	-2.934439	3.606643	-1.223099	1655.2736	1660.6545	3156.4497
	H	-4.785297	-0.697827	-0.762207	3158.5913	3158.9457	3160.5277
	H	-4.318459	1.652136	-1.354734	3162.3374	3166.0309	3172.7283
	H	-2.844419	-3.394232	-0.864651	3174.1360	3176.2932	3177.6413
	H	-4.222828	-2.650543	0.561579	3179.1480	3180.8597	3186.9353
	H	0.162863	-0.696496	1.733472	3189.6267	3220.5486	3220.9422
	H	-0.522966	-2.815496	2.716032			
	H	-2.678119	-3.875929	2.065111			
	C	-1.836162	-1.007857	0.307970	-598.7187	43.8518	57.5766
	C	-2.885151	-1.869938	-0.133364	68.8191	95.1318	117.3405
	C	-0.904596	-1.545390	1.230430	143.3634	167.0285	197.8639
	C	-1.849078	0.397581	-0.088252	228.7999	246.3347	269.0642
	C	-2.871515	-3.237595	0.229528	283.1810	292.6615	328.4338
	C	-3.992343	-1.327115	-0.855737	336.6596	360.5951	396.1731
	C	-0.936887	-2.871687	1.604047	413.0157	415.6165	443.7356
	C	-3.075797	0.909249	-0.594276	453.6525	478.3589	498.7889
	C	-1.908068	-3.740212	1.073102	505.4622	521.4989	535.6151
	C	-4.111122	0.015520	-1.014439	536.9718	554.3449	565.7117
	C	-0.750153	1.322737	0.073672	591.4450	614.4992	635.2021
	C	-3.292818	2.310465	-0.657097	641.4508	650.2561	693.2117
	C	-1.051703	2.705408	0.151659	704.2529	715.2575	749.7561
	C	-2.341803	3.177284	-0.203325	756.1037	759.4680	771.1645
	C	-0.046842	3.644658	0.567845	782.8785	783.9031	798.1281
TS **[i20]-p8**	C	1.229883	3.260589	0.801643	811.3637	814.9241	831.9746
	C	0.669114	0.957410	0.063642	842.6273	855.7271	870.7630
	C	1.649087	1.923067	0.497319	884.5049	900.1993	908.6295
	C	1.144001	-0.240241	-0.475339	925.4012	934.7521	951.0415
	C	2.502892	-0.573046	-0.490226	961.9197	968.6401	974.7951
	C	3.460666	0.341807	0.061281	978.0712	981.4743	996.7063
	C	3.000746	1.581405	0.522634	998.5856	1035.9102	1052.3186
	C	2.974932	-1.810732	-1.044143	1072.9419	1096.8906	1139.1305
	C	4.835990	-0.031923	0.090913	1162.1463	1165.9815	1175.7915
	C	4.309666	-2.156945	-0.940339	1181.9555	1183.9261	1191.4860
	C	5.244650	-1.252653	-0.385560	1210.3485	1211.9365	1230.0864
	H	-0.159056	-0.897830	1.667998	1241.2971	1249.9162	1287.0348
	H	-3.663034	-3.878825	-0.144134	1290.1010	1303.0652	1324.0269
	H	-4.770373	-1.999207	-1.201440	1355.0511	1360.6396	1366.2291
	H	-0.213490	-3.242623	2.321295	1372.7374	1398.4739	1406.9804
	H	-1.916963	-4.786767	1.355638	1418.5327	1442.0904	1448.4634

	H	-4.998218	0.441966	-1.470555	1460.0322	1471.2746	1505.9541
	H	-4.248248	2.673728	-1.019739	1507.6880	1536.2877	1543.6282
	H	-2.536051	4.243576	-0.162867	1565.5156	1579.8847	1615.9314
	H	-0.345777	4.678679	0.703258	1617.0984	1648.1798	1652.9370
	H	1.972090	3.972546	1.146034	1656.8953	1661.8567	3155.7475
	H	0.447373	-0.943238	-0.910447	3157.3118	3158.7994	3159.6714
	H	3.719898	2.315531	0.872738	3160.9186	3162.0061	3170.5245
	H	2.967026	-1.342350	-3.005548	3170.6436	3176.8345	3177.9719
	H	2.245306	-2.540879	-1.373974	3179.4811	3180.2790	3185.8112
	H	5.555752	0.663641	0.509502	3190.7502	3205.1559	3218.4838
	H	4.646929	-3.117827	-1.311099			
	H	6.291307	-1.531182	-0.338191			
	C	1.718317	1.204758	0.330784			
	C	2.498060	2.285956	-0.182260	18.5644	21.7441	47.5315
	C	0.874063	1.484334	1.434502	67.6184	78.8273	101.4027
	C	1.923306	-0.139240	-0.196253	117.8817	141.3913	172.8350
	C	2.291390	3.597085	0.309055	196.3064	214.2211	243.4099
	C	3.545555	2.021600	-1.116241	256.7076	292.7446	318.3422
	C	0.722703	2.763077	1.925249	327.5799	375.9620	389.0037
	C	3.117040	-0.364149	-0.931504	410.2701	420.5195	426.9711
	C	1.409804	3.840909	1.336337	442.2997	457.7955	463.9847
	C	3.881514	0.741246	-1.419854	478.7043	493.1256	508.7364
	C	1.057441	-1.274917	0.050860	540.3914	543.4876	550.8212
	C	3.581639	-1.690294	-1.152153	559.2506	598.3144	615.0895
	C	1.627174	-2.573301	-0.037602	633.1441	640.2246	645.9400
	C	2.907122	-2.752960	-0.631587	668.7469	689.1185	694.0600
	C	0.901758	-3.712517	0.430716	721.0264	731.2292	757.1808
	C	-0.375881	-3.600003	0.878780	762.6572	777.2769	792.7445
	C	-0.378640	-1.201947	0.290464	801.5330	813.8115	829.5914
	C	-1.069204	-2.358460	0.759943	834.8040	846.8709	863.2342
	C	-1.164452	-0.070690	-0.046478	877.0300	883.9304	885.7651
	C	-2.528075	-0.024196	0.163156	926.8810	947.0425	960.3357
	C	-3.174771	-1.144312	0.734246	967.4709	970.7587	978.4761
[i14]	C	-2.460262	-2.283141	1.012753	981.4528	984.6069	998.4142
	C	-3.339809	1.199557	-0.228121	1025.6284	1055.3326	1087.3548
	C	-4.305954	0.920452	-1.349934	1093.4185	1142.6810	1153.5944
	C	-5.654854	1.154756	-1.269152	1167.7085	1175.2982	1180.8422
	C	-6.855435	1.366924	-1.186005	1182.9819	1185.9008	1199.6142
	H	0.349719	0.672865	1.917779	1209.3729	1227.1186	1234.2535
	H	2.873711	4.406576	-0.118693	1241.1049	1250.8322	1287.7022
	H	4.115372	2.855196	-1.512510	1296.7364	1299.9184	1340.0283
	H	0.077807	2.935201	2.779614	1358.4371	1369.7089	1375.0018
	H	1.271849	4.847471	1.714485	1398.1680	1400.3247	1412.8430
	H	4.741702	0.529515	-2.046091	1430.8884	1449.1141	1464.2688
	H	4.513249	-1.831923	-1.689246	1471.2431	1474.2025	1512.3107
	H	3.304376	-3.758752	-0.715171	1527.5407	1548.1180	1552.4661
	H	1.401321	-4.675404	0.420700	1586.5456	1621.4689	1648.0253
	H	-0.911261	-4.464385	1.256707	1652.7043	1655.2102	1661.2071
	H	-0.683369	0.784776	-0.499645	2013.3594	3005.2962	3062.5064
	H	-4.243779	-1.110783	0.915065	3150.6991	3156.7231	3157.1182
	H	-2.963415	-3.162213	1.402057	3158.7430	3159.4198	3161.3735
	H	-2.649677	1.996819	-0.531488	3169.8766	3175.7299	3176.6649
	H	-3.891771	1.574587	0.638608	3177.7267	3179.8488	3185.4443
	H	-3.903887	0.505515	-2.269445	3203.8604	3216.7819	3468.9873
	H	-7.899241	1.551776	-1.120926			
	C	1.677798	1.270550	0.306401	25.0480	41.0406	59.3529
	C	2.428221	2.383769	-0.181419	70.7390	76.2766	115.0370
	C	0.749120	1.524219	1.346784	122.3558	135.7618	168.5155
	C	1.990648	-0.069988	-0.174961	192.2120	218.6957	242.6439
	C	2.117851	3.690714	0.264271	255.8402	276.8330	313.5555
	C	3.547093	2.160789	-1.040333	328.0042	350.3126	379.7982
	C	0.495122	2.802042	1.795695	408.1772	423.8017	426.8716
[i13]	C	3.239705	-0.241199	-0.828419	459.7100	473.3184	484.3937
	C	1.158699	3.904874	1.226620	506.2451	522.2352	538.2843
	C	3.972081	0.895816	-1.292479	540.9276	551.4873	557.1143
	C	1.175013	-1.247857	0.042662	594.2526	604.2666	616.8746
	C	3.789775	-1.542996	-0.990060	639.2049	664.9306	688.5654
	C	1.819336	-2.513958	0.017854	694.9319	720.4186	734.3297
	C	3.142696	-2.632271	-0.490448	748.0767	756.4324	760.1998
	C	1.129368	-3.683086	0.464004	776.6048	791.0411	797.8879

	C	-0.178807	-3.634128	0.830480	810.9180	818.2998	823.7245
	C	-0.275430	-1.251509	0.192359	837.7384	849.3948	864.1960
	C	-0.929045	-2.436506	0.644589	878.2130	884.5224	928.4440
	C	-1.098241	-0.175479	-0.217227	930.1927	941.5232	948.3349
	C	-2.477766	-0.200417	-0.091519	960.4220	967.5422	971.5150
	C	-3.095754	-1.344942	0.470480	979.0958	981.7480	988.7504
	C	-2.336719	-2.433238	0.812464	999.0689	1054.8561	1082.4859
	C	-3.266300	0.958431	-0.553280	1087.7526	1097.1681	1152.3445
	C	-4.566951	1.088517	-0.503345	1168.3555	1175.1384	1181.0253
	C	-5.904152	1.257115	-0.455929	1184.1061	1191.0041	1201.3129
	C	-6.807124	0.898502	-1.455321	1209.8258	1228.6414	1234.2213
	H	0.239302	0.694796	1.814788	1240.4329	1250.3096	1286.7415
	H	2.681239	4.523058	-0.144569	1293.9507	1301.3722	1340.5629
	H	4.094444	3.017380	-1.418846	1358.7378	1370.8977	1374.4210
	H	-0.214123	2.954485	2.601324	1396.0523	1399.6912	1413.9850
	H	0.940448	4.909470	1.570648	1438.5321	1449.4010	1466.8504
	H	4.881207	0.720881	-1.857994	1472.5311	1490.5101	1511.9550
	H	4.760379	-1.641678	-1.464006	1527.1979	1547.0196	1551.9670
	H	3.599090	-3.615515	-0.527004	1585.3318	1620.1027	1647.9159
	H	1.680027	-4.616839	0.504541	1651.1186	1652.2339	1660.4443
	H	-0.688546	-4.520593	1.192383	1885.4394	3063.0762	3094.0679
	H	-0.640543	0.696159	-0.663564	3149.5883	3156.8853	3157.5945
	H	-4.172969	-1.363617	0.590431	3159.0946	3160.0745	3161.4995
	H	-2.812748	-3.332238	1.190299	3170.5365	3176.3224	3177.3468
	H	-2.680875	1.779769	-0.973421	3179.7775	3181.6437	3185.6929
	H	-6.306371	1.714031	0.449130	3205.3241	3217.1607	3250.4570
	H	-6.470191	0.441855	-2.377024			
	H	-7.867211	1.072006	-1.326652			
	C	0.939665	1.545147	0.461017	19.0671	27.6421	56.6705
	C	1.115046	2.885361	0.001335	66.3087	73.5630	88.2452
	C	0.009688	1.339601	1.511693	121.6370	141.5065	158.6671
	C	1.797667	0.492672	-0.062492	188.8673	200.2000	235.7800
	C	0.252098	3.905959	0.465173	259.4959	280.3347	313.4936
	C	2.221683	3.202665	-0.844374	325.9152	349.7671	373.4445
	C	-0.789939	2.362554	1.981502	413.4822	419.7080	428.7642
	C	2.985315	0.898356	-0.725608	440.4128	472.9397	475.6687
	C	-0.701106	3.650338	1.424873	484.6163	510.5167	536.0790
	C	3.156821	2.260018	-1.128360	540.8248	552.1992	554.8118
	C	1.541231	-0.926247	0.057598	602.3709	619.0935	635.0922
	C	4.012662	-0.046710	-0.995312	662.2082	663.2621	674.3707
	C	2.616147	-1.829536	-0.153573	685.2755	691.6559	718.0702
	C	3.863080	-1.354254	-0.644552	725.2123	756.0822	762.9177
	C	2.439776	-3.233107	0.057854	770.3582	775.4873	788.5539
	C	1.225345	-3.761789	0.359550	796.5067	812.9923	832.3905
	C	0.221131	-1.509319	0.246575	839.4448	843.2900	860.7661
	C	0.069671	-2.926976	0.408658	879.2365	882.5974	942.2142
	C	-0.981008	-0.807598	0.181402	952.7229	960.2516	965.1760
	C	-2.251195	-1.285567	0.311332	967.7752	974.0043	976.4487
[i16]	C	-2.355589	-2.688325	0.518095	981.1289	994.0255	1008.4973
	C	-1.226913	-3.474336	0.564649	1024.6539	1059.0139	1083.6104
	C	-3.477408	-0.408307	0.198225	1102.7684	1148.8925	1167.8327
	C	-5.154247	0.560950	-1.393699	1169.1044	1179.9244	1180.8542
	C	-6.145661	1.236224	-1.467940	1185.0414	1208.4659	1209.9092
	C	-3.951921	-0.257566	-1.270027	1229.5271	1236.4588	1242.7282
	H	-0.030199	0.380480	2.005244	1259.2743	1286.5477	1292.4279
	H	0.381935	4.909834	0.074593	1308.5643	1332.2435	1349.8092
	H	2.338117	4.223942	-1.190784	1360.1729	1365.7292	1377.6229
	H	-1.475497	2.172642	2.799601	1389.4969	1404.1325	1412.2271
	H	-1.346734	4.444501	1.782049	1448.0797	1454.9773	1467.8640
	H	4.048398	2.517612	-1.690080	1476.4381	1492.5214	1497.8667
	H	4.928565	0.301273	-1.460652	1519.4457	1534.9054	1547.5618
	H	4.666574	-2.066079	-0.799432	1573.9392	1615.7486	1644.6316
	H	3.306807	-3.876012	-0.050496	1649.9362	1653.3194	1661.5918
	H	1.106547	-4.829106	0.513586	2220.1610	3024.0322	3046.7062
	H	-3.338538	-3.135412	0.635667	3055.9272	3097.4701	3147.5533
	H	-1.318871	-4.545485	0.709066	3157.0061	3157.8538	3159.9368
	H	-3.262693	0.583940	0.599774	3161.4461	3170.5763	3171.9409
	H	-4.292203	-0.832099	0.791670	3176.0786	3177.4198	3179.9494
	H	-7.020640	1.833446	-1.544242	3186.1773	3220.7031	3478.2418

	H	-4.140760	-1.249055	-1.696076			
	H	-3.143033	0.184329	-1.861047			
	C	1.442180	1.357275	0.405660			
	C	1.981075	2.591587	-0.069805	21.9435	32.2523	56.0146
	C	0.621980	1.413171	1.560436	67.0422	81.7585	84.9534
	C	1.861740	0.106454	-0.215764	120.4195	142.7838	156.0335
	C	1.564105	3.811993	0.513127	187.0635	209.0289	248.2902
	C	3.007187	2.579378	-1.062998	251.5574	292.9694	313.8944
	C	0.264897	2.612218	2.138110	327.5159	351.3713	378.9671
	C	3.034800	0.149178	-1.014810	408.7263	418.0485	422.5216
	C	0.709374	3.830070	1.590609	441.9664	453.9004	478.4107
	C	3.555755	1.403228	-1.462947	490.5324	502.9594	536.3314
	C	1.233479	-1.182682	-0.006716	541.8480	548.7233	559.5629
	C	3.722407	-1.052476	-1.341001	609.5358	616.7897	637.4633
	C	2.026680	-2.344647	-0.202815	659.1120	664.4920	675.4345
	C	3.283819	-2.249443	-0.861631	684.5810	692.1985	719.0526
	C	1.550721	-3.622603	0.224401	722.8492	757.4526	762.3802
	C	0.302148	-3.777273	0.737813	770.0163	774.9765	784.8922
	C	-0.177291	-1.391100	0.300112	796.0442	812.2274	831.6712
	C	-0.611878	-2.682495	0.728841	839.4828	851.1997	868.8885
	C	-1.166946	-0.402175	0.062530	878.6173	884.9297	913.2311
	C	-2.514514	-0.601739	0.328728	944.8819	957.4850	963.5839
	C	-2.838839	-1.853650	0.850398	968.4050	968.9038	975.6256
[i15]	C	-1.985656	-2.885688	1.049487	981.0527	999.0780	1016.3631
	C	-3.557938	0.451745	0.041425	1025.1967	1055.1799	1081.5388
	C	-5.520998	1.051433	-1.396036	1096.0170	1155.3826	1168.0847
	C	-6.353997	1.892778	-1.602142	1175.7707	1180.4595	1184.1006
	C	-4.496534	0.048357	-1.123005	1191.2969	1205.0376	1221.2466
	H	0.282909	0.493016	2.013649	1229.5457	1233.8662	1244.7771
	H	1.963710	4.738216	0.113514	1271.0579	1284.6157	1287.9877
	H	3.391758	3.525331	-1.428832	1307.3740	1324.4914	1353.9643
	H	-0.353789	2.613611	3.028379	1362.3952	1368.8892	1375.4227
	H	0.408969	4.770751	2.037776	1391.9428	1397.7210	1411.0746
	H	4.404915	1.390905	-2.137939	1438.7151	1450.0109	1467.4638
	H	4.633665	-0.987566	-1.925556	1476.6176	1491.7174	1497.8396
	H	3.854061	-3.157220	-1.026247	1511.8964	1539.2451	1546.1422
	H	2.217644	-4.473165	0.131265	1578.1191	1611.0546	1630.8774
	H	-0.042144	-4.745297	1.084956	1648.2436	1652.0656	1659.9399
	H	-0.869745	0.548243	-0.360431	2220.9202	3023.0636	3043.4503
	H	-2.313422	-3.857437	1.404587	3052.9364	3092.5361	3157.2218
	H	-3.070479	1.398846	-0.199807	3157.6373	3159.3353	3160.1139
	H	-4.166169	0.622065	0.934564	3162.1637	3170.6298	3177.0109
	H	-7.094016	2.630851	-1.791252	3178.3267	3180.4405	3186.1395
	H	-4.974410	-0.907952	-0.884614	3194.8279	3216.2365	3478.1224
	H	-3.899998	-0.120554	-2.026052			
	C	1.565275	-0.566134	-0.478362	49.3213	66.5359	68.1985
	C	2.792393	-1.228429	-0.172419	102.1673	112.0989	125.2185
	C	0.700074	-1.198258	-1.403584	161.3587	177.1034	232.1915
	C	1.316302	0.762747	0.067262	247.1725	248.8901	286.5666
	C	3.039146	-2.522874	-0.686084	317.4315	325.5031	369.2263
	C	3.797047	-0.546558	0.580858	390.9293	403.6550	418.2041
	C	0.982932	-2.442680	-1.924366	424.5090	436.9447	473.5304
	C	2.431260	1.463705	0.601336	486.5786	498.6997	515.6295
	C	2.148082	-3.130649	-1.540250	516.8433	538.3626	545.9669
	C	3.643239	0.764768	0.898664	556.5992	575.2175	606.0625
	C	0.049095	1.457294	-0.003686	619.1287	652.2982	668.3422
	C	2.362469	2.869472	0.794722	684.9535	696.3837	720.5515
[i17]	C	0.085769	2.878615	-0.020264	735.9414	747.8877	755.8139
	C	1.257998	3.564146	0.397217	769.4824	777.9851	792.1887
	C	-1.050724	3.617819	-0.474701	807.7899	816.4752	832.6909
	C	-2.185452	2.980951	-0.861674	838.7363	841.7708	857.6704
	C	-1.267660	0.828704	-0.055646	860.2119	882.9630	896.1665
	C	-2.345289	1.580864	-0.620699	924.2941	932.3804	954.3605
	C	-1.583987	-0.439505	0.529057	960.0933	964.9058	972.9789
	C	-2.839709	-1.022031	0.309824	978.2047	983.2905	989.7943
	C	-3.816843	-0.331168	-0.424652	994.1461	1017.6462	1048.9525
	C	-3.592019	0.960965	-0.841955	1060.5514	1104.3537	1128.1135
	C	-3.198854	-2.338862	0.974190	1165.2045	1169.5850	1170.2242
	C	-0.896171	-2.415059	1.735730	1178.3321	1184.3105	1189.3497
	C	-0.670678	-1.143437	1.464047	1194.5555	1211.2601	1218.3621

	C	-1.981912	-3.263586	1.199014	1232.9309	1238.5705	1244.6936
	H	-0.194478	-0.687253	-1.727762	1248.4053	1274.8154	1296.7389
	H	3.967105	-3.017182	-0.417875	1324.7693	1334.1741	1340.8169
	H	4.712724	-1.073758	0.826444	1361.0835	1363.0613	1369.5949
	H	0.304701	-2.887930	-2.643805	1394.3878	1401.4721	1416.4453
	H	2.356088	-4.116931	-1.939463	1445.4803	1451.1416	1463.4553
	H	4.443831	1.313929	1.382907	1467.7335	1473.1562	1505.1742
	H	3.231481	3.384655	1.189499	1522.7505	1544.4115	1552.6969
	H	1.241836	4.648262	0.428568	1579.5698	1608.7297	1629.6841
	H	-0.966776	4.697023	-0.544850	1648.0388	1651.6112	1658.7614
	H	-3.021039	3.533519	-1.277620	1685.2286	2990.8265	2999.5997
	H	-4.780694	-0.798812	-0.598038	3056.5208	3059.0290	3154.7109
	H	-4.382998	1.531750	-1.316473	3156.1285	3157.9349	3158.8075
	H	-3.962917	-2.857500	0.387558	3160.9396	3167.7948	3173.6017
	H	-3.647503	-2.117197	1.952151	3175.9351	3176.3134	3177.7152
	H	0.152597	-0.594475	1.904293	3179.5922	3184.0022	3219.1510
	H	-1.654900	-3.723634	0.256423			
	H	-2.249759	-4.079382	1.876566			
	C	-1.784498	-1.031551	0.295926			
	C	-2.816968	-1.920161	-0.134374	44.1492	56.9291	68.7982
	C	-0.820106	-1.550396	1.196188	92.9950	113.7850	137.2951
	C	-1.844440	0.374257	-0.085550	159.1407	186.3721	211.7843
	C	-2.756466	-3.290353	0.215048	237.6924	271.2311	284.9515
	C	-3.950547	-1.402030	-0.831295	317.8953	322.1476	351.2333
	C	-0.807975	-2.880070	1.557914	381.4247	404.7585	413.5875
	C	-3.091409	0.856442	-0.563470	426.4264	442.2768	454.0517
	C	-1.763620	-3.771932	1.036240	482.1910	499.2879	503.0580
	C	-4.108401	-0.060736	-0.974764	534.6308	548.7411	553.1738
	C	-0.765644	1.329837	0.073931	558.8086	579.1108	615.0192
	C	-3.352270	2.254502	-0.597318	624.8443	645.7358	680.7356
	C	-1.110730	2.704212	0.187966	691.1391	700.8940	724.9613
	C	-2.424201	3.140322	-0.139480	742.6243	752.5393	758.0684
	C	-0.128431	3.661627	0.587835	770.9927	777.5869	794.9766
	C	1.169608	3.305400	0.775310	803.9407	813.8551	825.3888
	C	0.652671	1.009049	0.034495	837.0631	841.3315	856.3911
	C	1.606053	1.988035	0.442484	884.0734	885.0837	902.8125
	C	1.163331	-0.192701	-0.524677	920.8689	927.7560	933.3833
	C	2.507905	-0.475181	-0.578241	947.7641	961.0432	967.5568
	C	3.444855	0.457527	-0.040256	974.2494	976.8267	979.9914
[i18]	C	2.983306	1.667291	0.435317	997.6922	1023.2101	1050.6982
	C	3.034056	-1.712529	-1.278464	1069.6560	1094.1564	1138.8905
	C	5.203592	-1.166016	-0.267547	1167.0621	1171.1949	1176.4597
	C	4.874914	0.089050	-0.016822	1180.3296	1183.8853	1199.3394
	C	4.305746	-2.293121	-0.604159	1204.4143	1208.1494	1229.4887
	H	-0.087190	-0.884053	1.627134	1232.2708	1243.8926	1247.8645
	H	-3.535939	-3.951129	-0.149916	1255.7521	1287.6820	1296.7494
	H	-4.716306	-2.091684	-1.169885	1319.1004	1331.6240	1348.9427
	H	-0.063167	-3.236165	2.260787	1359.9200	1373.9554	1380.1555
	H	-1.737749	-4.820583	1.310004	1394.7088	1409.0560	1419.5320
	H	-5.015486	0.345129	-1.410026	1448.9219	1466.9029	1469.0566
	H	-4.324992	2.593633	-0.936729	1476.7326	1477.5618	1509.5999
	H	-2.650866	4.199092	-0.075023	1515.1870	1538.9341	1549.1923
	H	-0.447050	4.687432	0.739845	1585.0628	1620.0006	1647.1378
	H	1.904032	4.033062	1.103602	1648.8860	1653.3064	1660.3455
	H	0.471014	-0.904465	-0.952891	1683.1906	2997.5037	3006.6910
	H	3.689894	2.408908	0.795524	3055.3258	3072.3533	3142.7047
	H	3.297824	-1.438627	-2.308090	3154.3624	3156.5442	3157.9859
	H	2.258362	-2.480023	-1.339295	3158.8657	3160.9580	3169.1843
	H	5.604058	0.847367	0.254553	3175.9326	3176.9404	3179.4353
	H	4.783608	-3.012519	-1.275739	3184.8580	3200.9323	3217.1607
	H	4.047973	-2.840014	0.312730			
	C	1.569760	-0.595259	-0.505409	46.2990	63.2215	66.6462
	C	2.788998	-1.279095	-0.213661	86.5241	104.2199	121.4995
	C	0.690024	-1.207757	-1.430526	138.1493	183.2207	223.4701
	C	1.338841	0.728486	0.060581	244.6569	251.8560	282.8034
[i19]	C	3.016825	-2.569691	-0.746240	312.9048	325.9006	366.0078
	C	3.804433	-0.624014	0.548559	404.1768	422.9843	424.0273
	C	0.953360	-2.449238	-1.967936	434.7367	460.0315	477.6302
	C	2.462802	1.401808	0.608815	489.4122	507.0592	515.5024
	C	2.112882	-3.155777	-1.601850	522.0327	541.3322	546.6725

	C	3.666412	0.682364	0.891602	566.2261	600.1407	615.4045
	C	0.078549	1.444630	-0.000237	624.3829	654.7900	673.2687
	C	2.417569	2.805069	0.831232	674.4563	687.6369	701.3450
	C	0.143407	2.867349	0.011356	727.8417	746.5162	754.4347
	C	1.326314	3.524623	0.445522	757.7310	774.3489	777.2393
	C	-0.977194	3.638729	-0.421261	807.2204	812.0041	814.0326
	C	-2.124635	3.031638	-0.819825	838.3121	839.2981	840.9634
	C	-1.246623	0.844420	-0.073031	858.0740	883.5447	905.2268
	C	-2.305569	1.629613	-0.616139	923.9505	933.4776	953.9154
	C	-1.591204	-0.451673	0.478719	956.2665	959.8966	965.3317
	C	-2.854591	-1.014142	0.180038	967.7094	972.3049	978.1504
	C	-3.806374	-0.272170	-0.532631	993.0392	996.0644	1041.4543
	C	-3.562835	1.037524	-0.877709	1059.8726	1102.7761	1105.1016
	C	-3.224411	-2.407962	0.646479	1139.0918	1165.5101	1171.1588
	C	-0.752606	-1.135304	1.412555	1178.1603	1180.8653	1184.4442
	C	-1.119481	-2.375461	1.973084	1193.5495	1201.6696	1203.1722
	C	-2.273284	-3.013067	1.627939	1215.5573	1232.5320	1242.3591
	H	-0.200195	-0.682040	-1.742672	1245.4654	1257.9664	1290.6084
	H	3.940425	-3.078507	-0.490160	1292.4450	1316.6499	1356.0446
	H	4.714052	-1.167005	0.782144	1359.5752	1368.9341	1380.9766
	H	0.262375	-2.878923	-2.684475	1387.7093	1406.5923	1413.9793
	H	2.305356	-4.139790	-2.014185	1431.5337	1445.7053	1449.3096
	H	4.473825	1.212806	1.385296	1463.5770	1469.4938	1504.2699
	H	3.294625	3.297313	1.237200	1523.2788	1541.2336	1548.5808
	H	1.326942	4.608023	0.498516	1566.1411	1581.6745	1602.9056
	H	-0.873792	4.717696	-0.463498	1623.3931	1648.6380	1650.6607
	H	-2.951480	3.608292	-1.220134	1659.7037	2918.1960	2974.1926
	H	-4.771057	-0.719813	-0.751285	3151.0814	3155.1521	3155.6942
	H	-4.339168	1.641520	-1.334575	3157.7456	3158.6682	3160.9327
	H	-3.309713	-3.067780	-0.235140	3168.7334	3173.3500	3175.4346
	H	-4.239867	-2.394707	1.068723	3175.6543	3177.8097	3179.7236
	H	0.160087	-0.666867	1.746381	3184.4729	3219.0313	3229.0603
	H	-0.454209	-2.827386	2.701666			
	H	-2.526441	-3.976689	2.056038			
[i20]	C	-1.824295	-1.017210	0.302824	41.3997	56.0857	68.8713
	C	-2.861569	-1.896160	-0.135454	81.3298	112.0383	119.0113
	C	-0.885423	-1.537713	1.228939	147.4786	195.6168	204.6553
	C	-1.854877	0.383463	-0.099514	232.7509	272.7009	282.1595
	C	-2.828766	-3.262012	0.234018	310.5648	333.9787	358.3630
	C	-3.972942	-1.370933	-0.862528	388.7252	411.6738	424.2465
	C	-0.900368	-2.862295	1.608934	442.8505	455.9865	477.0495
	C	-3.084465	0.877985	-0.609425	488.9556	501.0285	515.8075
	C	-1.859302	-3.746946	1.080813	534.7916	549.4044	555.1081
	C	-4.107032	-0.029716	-1.028511	569.0543	605.5187	612.4927
	C	-0.764681	1.324628	0.069323	624.2770	646.0371	664.8515
	C	-3.322456	2.278780	-0.667323	676.3524	692.7580	702.5220
	C	-1.091650	2.705700	0.160100	725.6561	744.9889	757.4919
	C	-2.389662	3.156746	-0.200900	767.9664	775.8367	781.7707
	C	-0.102595	3.653818	0.571714	795.0521	802.6133	814.3965
	C	1.184375	3.281618	0.791482	830.9880	841.1276	854.5097
	C	0.647653	0.982354	0.060961	883.8904	887.8917	898.0834
	C	1.610816	1.952317	0.481630	906.1599	926.1305	943.5427
	C	1.152058	-0.232427	-0.471247	954.7902	959.5595	962.1722
	C	2.491205	-0.544179	-0.492536	967.3583	967.7256	974.0155
	C	3.443313	0.380501	0.047826	979.5037	998.4214	1048.3196
	C	2.974029	1.612832	0.504320	1060.8792	1086.9495	1103.6609
	C	2.960923	-1.854849	-1.097099	1151.2280	1168.8049	1172.3002
	C	4.831706	0.039252	0.073259	1175.5033	1183.4502	1188.5328
	C	4.432267	-2.109678	-0.976787	1195.1189	1205.2761	1209.0114
	C	5.286589	-1.194802	-0.424554	1227.5125	1232.4680	1244.6735
	H	-0.151205	-0.876222	1.665194	1256.0288	1287.9989	1298.2552
	H	-3.610902	-3.916170	-0.137145	1313.6065	1322.9012	1351.1490
	H	-4.742334	-2.053768	-1.206681	1359.9126	1371.6094	1382.1205
	H	-0.174741	-3.219593	2.330997	1396.3485	1412.5268	1422.1045
	H	-1.854492	-4.791998	1.369110	1445.1748	1447.6611	1450.3196
	H	-4.998761	0.383486	-1.487958	1462.8540	1472.1639	1509.0056
	H	-4.282203	2.628646	-1.031805	1519.9262	1537.5077	1547.5516
	H	-2.601633	4.219545	-0.154913	1563.2917	1581.2347	1615.0010
	H	-0.410179	4.685335	0.707130	1628.4351	1647.6706	1651.0866
	H	1.922285	4.001742	1.128429	1659.0218	2954.3213	2979.2551

	H	0.455172	-0.941273	-0.898230	3152.4589	3153.9668	3156.4061
	H	3.687461	2.351423	0.857152	3157.7328	3158.7363	3160.8234
	H	2.675178	-1.887210	-2.160685	3169.2806	3170.5168	3175.8216
	H	2.403796	-2.687116	-0.642854	3176.8227	3179.2650	3181.4264
	H	5.536074	0.750384	0.489387	3184.9124	3194.8155	3216.8007
	H	4.810872	-3.051655	-1.358237			
	H	6.346503	-1.421998	-0.370468			
	C	-1.581890	-0.372869	0.177977			
	C	-2.957272	-0.285639	-0.197950	65.3040	72.5384	90.7471
	C	-1.178361	-1.532164	0.886471	120.1284	172.3097	177.5815
	C	-0.703902	0.768253	-0.051702	231.5048	245.1348	278.6399
	C	-3.812709	-1.394930	0.002923	312.7345	343.6403	399.4229
	C	-3.480929	0.951013	-0.683520	413.1155	419.6204	449.9144
	C	-2.042067	-2.582438	1.108842	469.9617	477.7598	496.8619
	C	-1.328488	2.016701	-0.310827	518.4395	537.8726	545.3093
	C	-3.365315	-2.532895	0.632896	552.2910	567.5281	611.6022
	C	-2.711139	2.069719	-0.671585	626.4803	650.8386	673.6535
	C	0.741240	0.745909	0.054486	691.4039	717.5980	727.5049
	C	-0.592741	3.226229	-0.173811	756.8321	763.7678	774.2370
	C	1.405240	1.968473	0.341765	782.4896	791.5643	809.3902
	C	0.705311	3.202296	0.238141	820.8017	838.1123	856.8251
	C	2.790088	1.971592	0.695968	859.9374	881.6039	884.6324
	C	3.527891	0.831854	0.670488	931.8493	944.8117	951.1480
	C	1.584765	-0.412359	-0.208775	962.5356	968.8668	976.1237
5_helicenyl	C	2.967676	-0.377038	0.155299	981.0937	998.6637	1047.8897
	C	1.138526	-1.548923	-0.948087	1062.8282	1082.1904	1091.5193
	C	2.011652	-2.566668	-1.156112	1143.2076	1160.8101	1172.8456
	C	3.331979	-2.622481	-0.732626	1178.7325	1184.1668	1201.0184
	C	3.802338	-1.497484	-0.080979	1215.1176	1228.7572	1233.3866
	H	-0.173977	-1.589579	1.279841	1244.4467	1268.0070	1287.1121
	H	-4.845662	-1.315554	-0.319555	1322.2534	1343.2164	1359.5375
	H	-4.522198	0.995542	-0.984097	1374.4292	1389.3832	1403.1462
	H	-1.699083	-3.448193	1.663870	1414.4826	1442.4288	1450.6335
	H	-4.034204	-3.370654	0.793765	1467.1466	1496.8366	1513.7062
	H	-3.131745	3.032885	-0.940390	1536.2778	1549.3033	1582.9360
	H	-1.103864	4.167284	-0.345851	1610.4618	1621.5994	1648.3456
	H	1.243841	4.123143	0.433936	1653.5807	1660.5992	3153.3998
	H	3.240140	2.914194	0.988523	3157.3643	3159.0921	3159.9179
	H	4.571917	0.839701	0.964301	3161.9091	3171.0204	3176.8089
	H	0.133470	-1.580643	-1.345424	3177.9722	3179.7908	3180.5051
	H	3.970161	-3.478193	-0.919630	3186.1317	3199.5361	3217.4037
	H	4.839841	-1.446831	0.235018			

Table S2.

Bimolecular reactions and degradation pathways incorporated into the astrochemical models.

R_1	R_2	P_1	P_2	α	β	γ	No.
C3H3	C3H3	C6H5	H	4.00E-10	0	0	1
C4H6	C2H	C6H6	H	4.00E-10	0	0	2
C2H4	C2H	C4H4	H	4.00E-10	0	0	3
C6H6	C	C6H5C	H	4.00E-10	0	0	4
C6H6	CH	C6H5CH	H	4.00E-10	0	0	5
C6H6	C2	C6H5C2	H	4.00E-10	0	0	6
C6H6	C2H	C6H5C2H	H	4.00E-10	0	0	7
C6H6	CN	C6H5CN	H	4.00E-10	0	0	8
C6H6	hv	C6H5	H	3.00E-09	0	3.1	9
C6H5	C4H4	C10H8	H	4.00E-10	0	0	10
C10H8	C	C10H7C	H	4.00E-10	0	0	11
C10H8	CH	C10H7CH	H	4.00E-10	0	0	12
C10H8	C2	C10H7C2	H	4.00E-10	0	0	13
C10H8	C2H	C10H7C2H	H	4.00E-10	0	0	14
C10H8	CN	C10H7CN	H	4.00E-10	0	0	15
C10H8	hv	C10H7	H	2.00E-09	0	3.1	16
C10H7	C4H4	C14H10	H	4.00E-10	0	0	17
C10H8	hv	C9H7C	H	2.00E-09	0	3.1	18
C9H7C	C4H4	C14H10	H	2.00E-10	0	0	19
C9H7C	C4H4	C13H10C	H	2.00E-10	0	0	20
C14H10	hv	C14H9	H	4.60E-09	0	3.1	21
C13H10C	hv	C13H9C	H	4.60E-09	0	3.1	22
C14H10	C	C14H9C	H	4.00E-10	0	0	23
C14H10	CH	C14H9CH	H	4.00E-10	0	0	24
C14H10	C2	C14H9C2	H	4.00E-10	0	0	25
C14H10	C2H	C14H9C2H	H	4.00E-10	0	0	26
C14H10	CN	C14H9CN	H	4.00E-10	0	0	27
C13H10C	C	C13H9CC	H	4.00E-10	0	0	28
C13H10C	CH	C13H9CCH	H	4.00E-10	0	0	29
C13H10C	C2	C13H9CC2	H	4.00E-10	0	0	30
C13H10C	C2H	C13H9CC2H	H	4.00E-10	0	0	31
C13H10C	CN	C13H9CCN	H	4.00E-10	0	0	32
C2	C4H6	C6H5	H	4.00E-10	0	0	33
C6H4CN	C4H4	C10H7CN	H	4.00E-10	0	0	34
C6H5CN	hv	C6H4CN	H	3.00E-09	0	3.1	35
C10H7CN	hv	C10H6CN	H	3.00E-09	0	3.1	36
C10H6CN	C4H4	C14H9CN	H	4.00E-10	0	0	37
C2H4	CH	CH2CCH2	H	4.00E-10	0	0	38
CH2CCH2	hv	C3H3	H	3.00E-09	0	3.1	39
C2H4	C	C3H3	H	4.00E-10	0	0	40
C2H6	hv	C2H4	H2	3.00E-09	0	3.1	41
C2H6	CH	C3H6	H	4.00E-10	0	0	42
C3H6	CH	C4H6	H	4.00E-10	0	0	43
C4H6	CH	C5H6	H	4.00E-10	0	0	44
C5H6	CN	C5H5CN	H	4.00E-10	0	0	45
C5H5CN	CH	C6H5CN	H	4.00E-10	0	0	46
C5H6	CH	C6H6	H	4.00E-10	0	0	47
C14H9	C4H4	C18H12	H	4.00E-10	0	0	48
C18H12	hv	C18H11	H	3.00E-09	0	3.1	49
C18H11	C4H4	C22H14	H	4.00E-10	0	0	50
C22H14	hv	C22H13	H	3.00E-09	0	3.1	51
C22H13	C4H4	C26H16	H	4.00E-10	0	0	52
C26H16	hv	C26H15	H	3.00E-09	0	3.1	53
C18H12	C	C18H11C	H	4.00E-10	0	0	54
C18H12	CH	C18H11CH	H	4.00E-10	0	0	55
C18H12	C2	C18H11C2	H	4.00E-10	0	0	56

C18H12	C2H	C18H11C2H	H	4.00E-10	0	0	57
C18H12	CN	C18H11CN	H	4.00E-10	0	0	58
C22H14	C	C22H13C	H	4.00E-10	0	0	59
C22H14	CH	C22H13CH	H	4.00E-10	0	0	60
C22H14	C2	C22H13C2	H	4.00E-10	0	0	61
C22H14	C2H	C22H13C2H	H	4.00E-10	0	0	62
C22H14	CN	C22H13CN	H	4.00E-10	0	0	63
C26H16	C	C26H15C	H	4.00E-10	0	0	64
C26H16	CH	C26H15CH	H	4.00E-10	0	0	65
C26H16	C2	C26H15C2	H	4.00E-10	0	0	66
C26H16	C2H	C26H15C2H	H	4.00E-10	0	0	67
C26H16	CN	C26H15CN	H	4.00E-10	0	0	68

Note: R1 and R2 are reactants, P1 and P2 are the products. Reaction rate coefficients and (preexponential) factors α (s^{-1}) are parameterized according to Section 2.1 of D. McElroy, C. Walsh, A. J. Markwick, M. A. Cordiner, K. Smith, T. J. Millar, The UMIST database for astrochemistry 2012, A&A, 550, A36 (2013). The in the table are given at 300 K.